

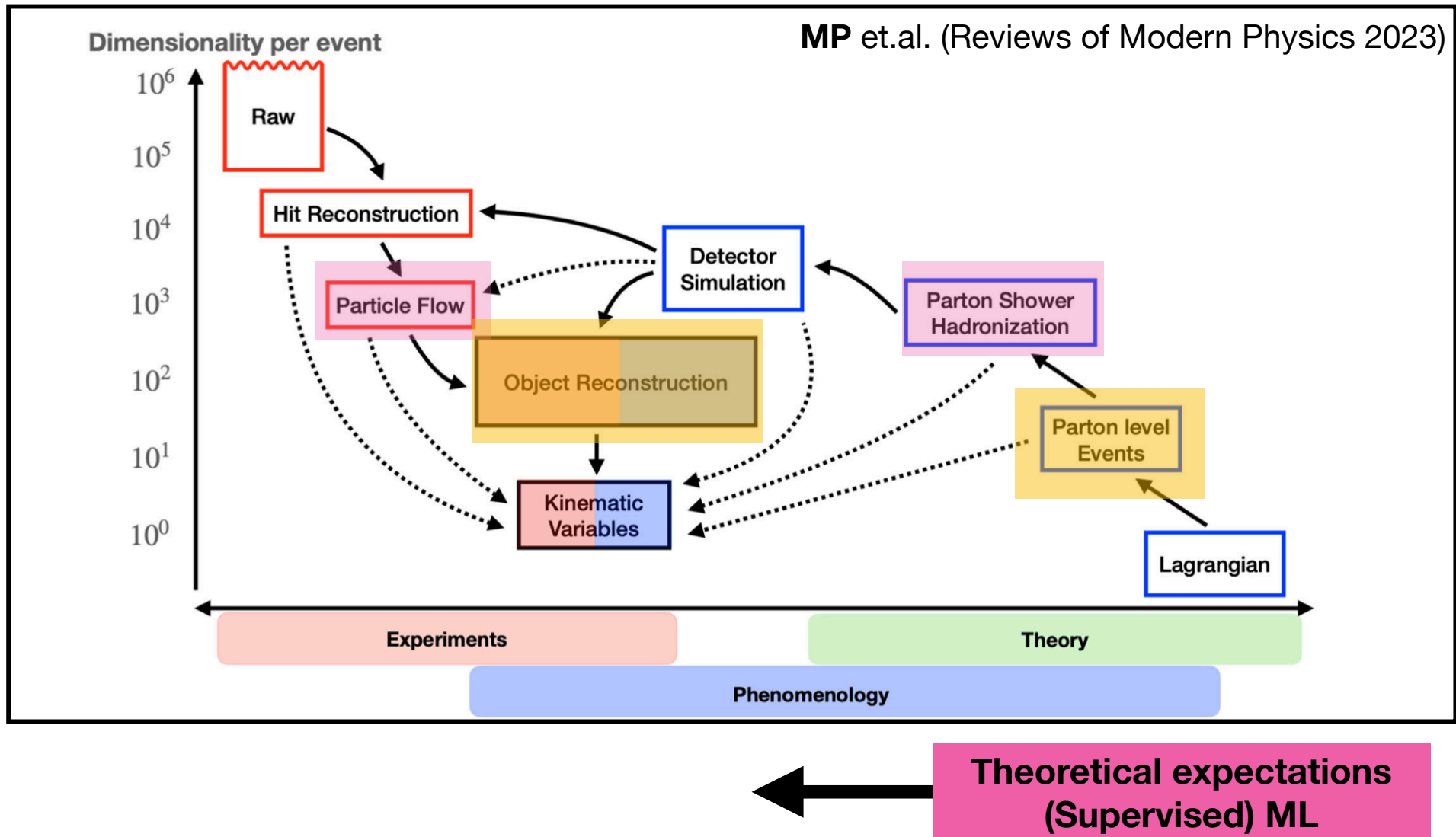
AI for Collider Physics
Efficient Computation
&
New Physics Discovery

Myeonghun Park
SeoulTech

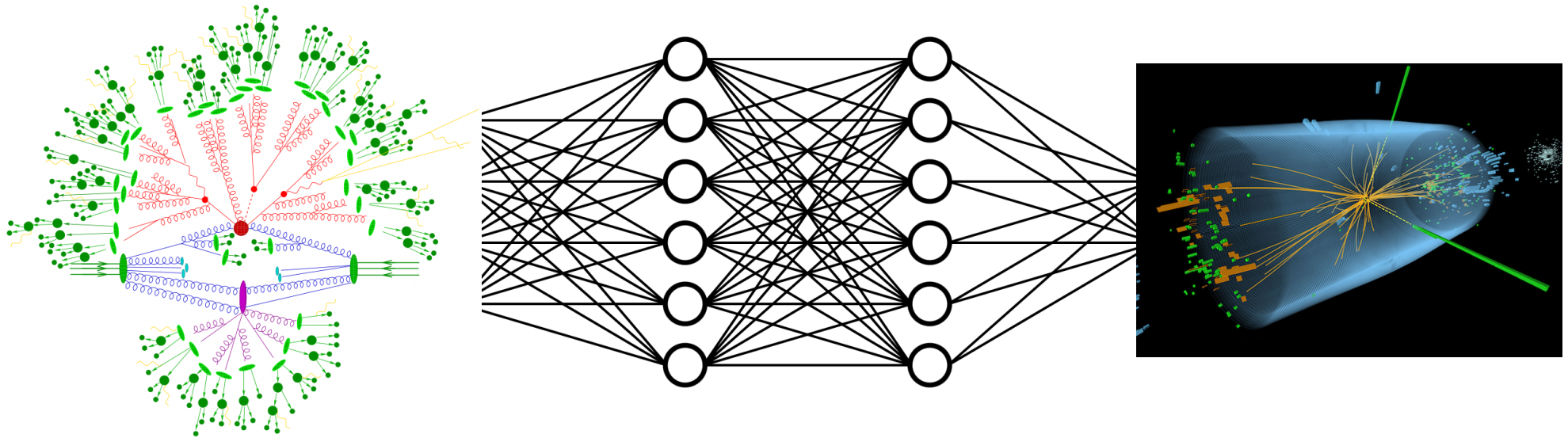
한국고에너지물리학회 2026 봄 학술대회
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Understanding Physics using the LHC

- Recent advancements in Machine Learning (ML) allow us to fully exploit **all available information**, including raw-level data such as detector responses.

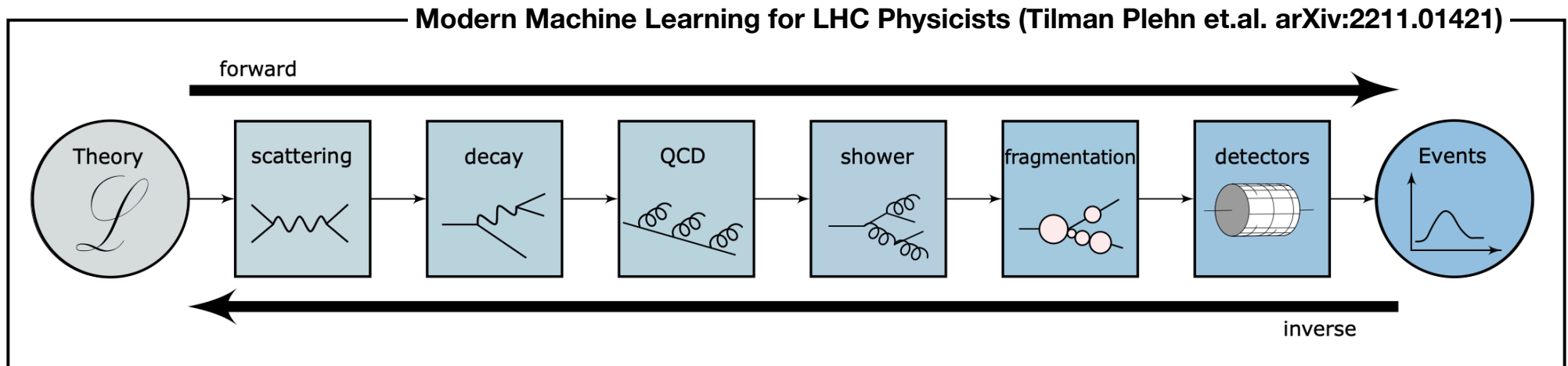


Theory-Compare-Data

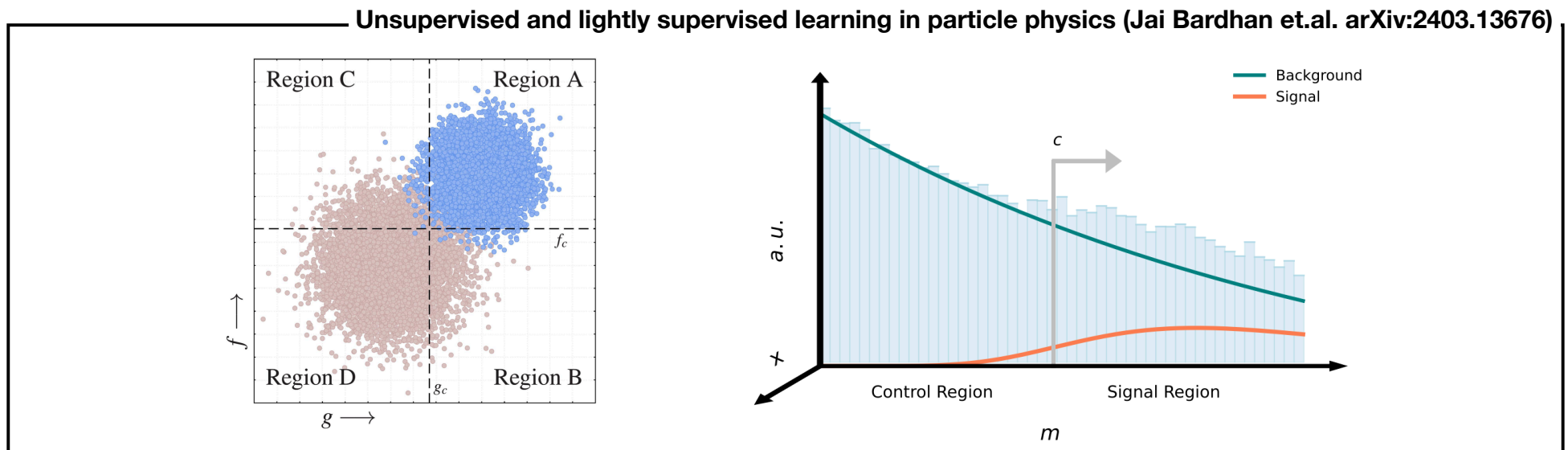


- With our elaborated **theoretical model**,
 - 1) Get **expectations** from **MC simulations**
 - 2) Get **data** from **experiments** (e.g. the LHC)
 - 3) Compare our expectation to data with sophisticated computer **algorithms** (including Machine Learning)

- Data come from the chain of **Monte Carlo simulations**

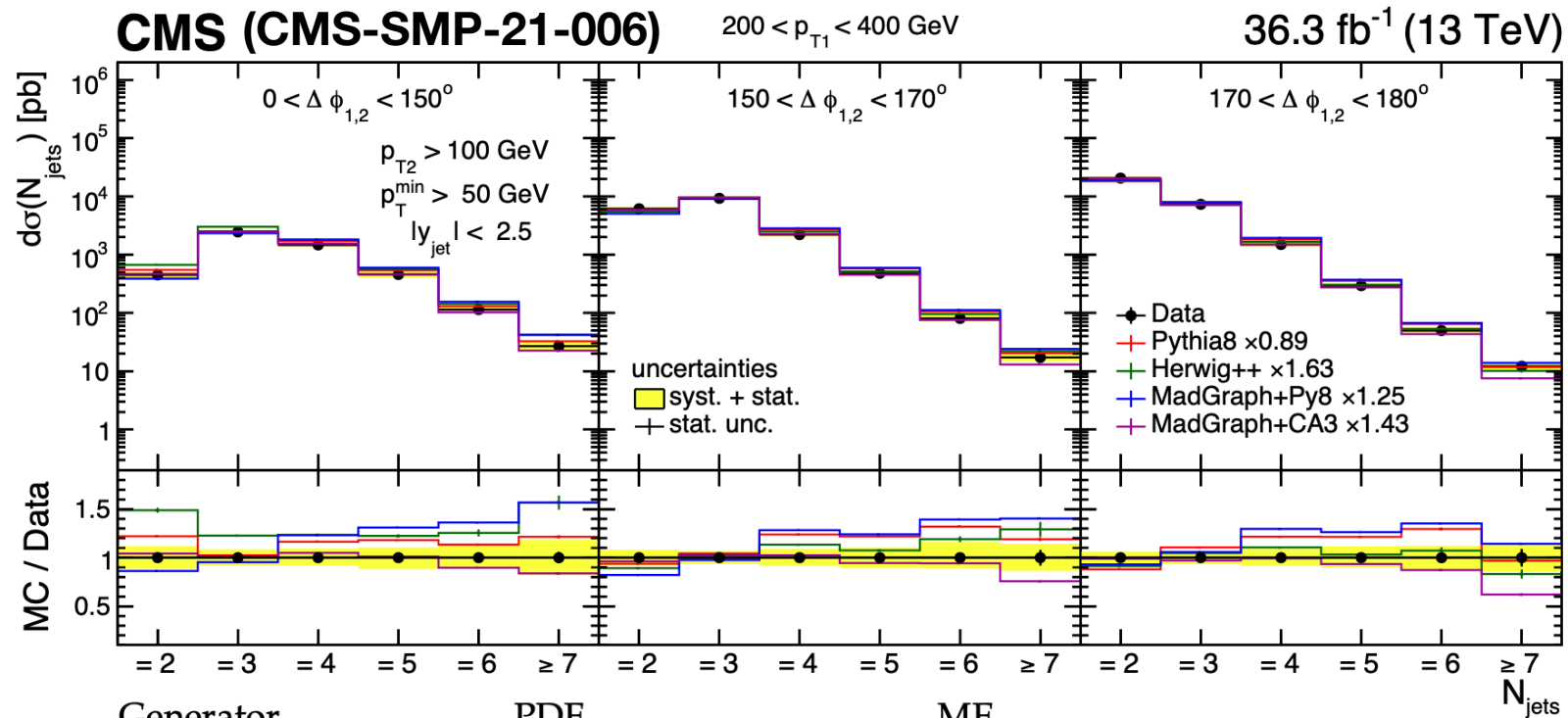


- Data come from **LHC data (controlled samples)**



Importance of Precision

- For Machine Learning which requires "training", the big amount of well-understood data is necessary.

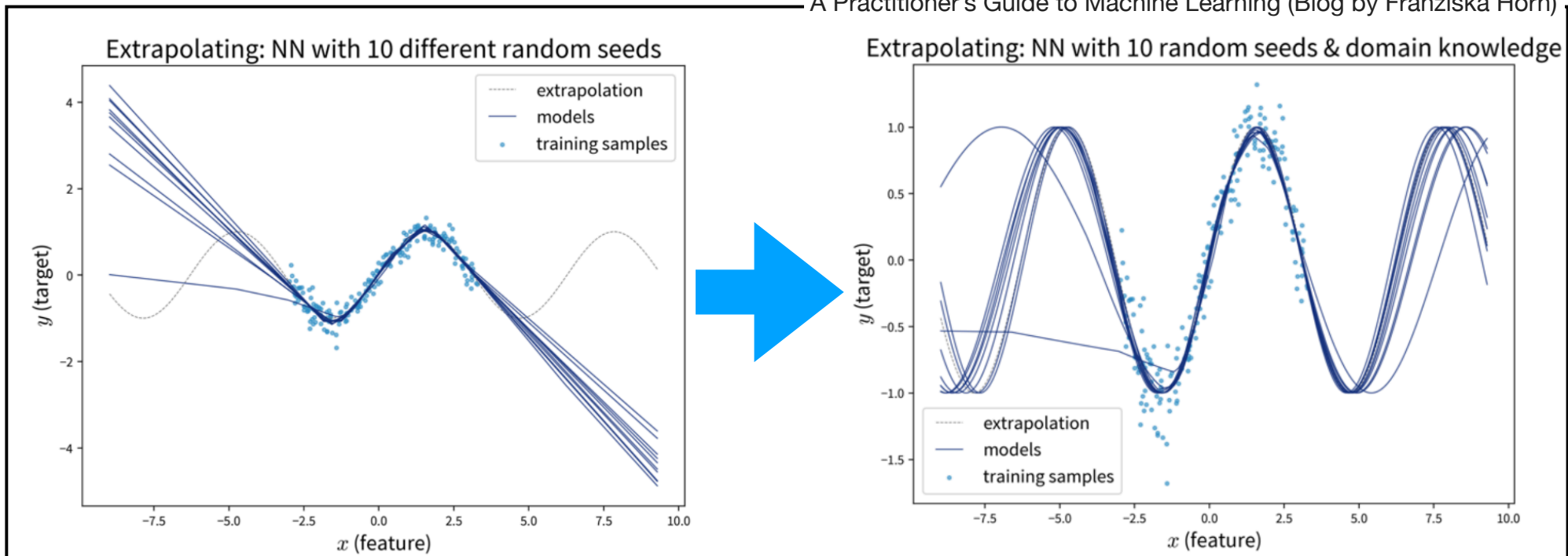


Generator	PDF	ME
PYTHIA8 [23]	NNPDF 2.3 (LO) [25]	LO $2 \rightarrow 2$
MADGRAPH+PY8 [4]	NNPDF 2.3 (LO) [25]	LO $2 \rightarrow 2, 3, 4$
MADGRAPH+CA3 [4]	PB-TMD set 2 (NLO) [1]	LO $2 \rightarrow 2, 3, 4$
HERWIG++ [26]	CTEQ6L1 (LO) [27]	LO $2 \rightarrow 2$

Importance of Theory

- We need **HUGE** "training data" to feed the "data hungry" Neural Net.
- One can dream of "data-driven" machine learning.
 - We cannot guarantee the estimation out of Controlled samples.
 - : **NO magic can do "Exploration".**
 - : **Domain knowledge is strongly required.**

A Practitioner's Guide to Machine Learning (Blog by Franziska Horn)



Region of the "LOW" statistics

- As we get a statistics,
we are approaching a high energy region
= **Huge multiplicity.**

$$gg \rightarrow gg$$

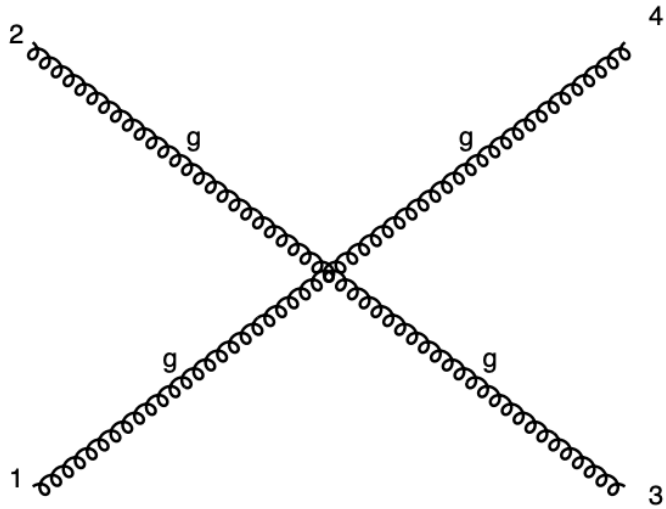


diagram 1

QCD=2, QED=0

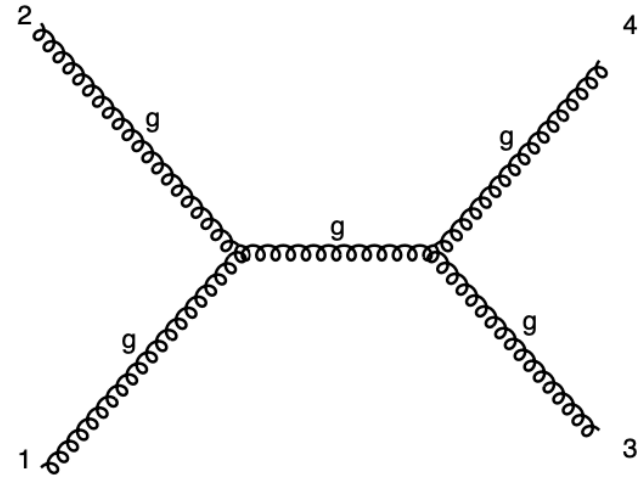


diagram 2

QCD=2, QED=0

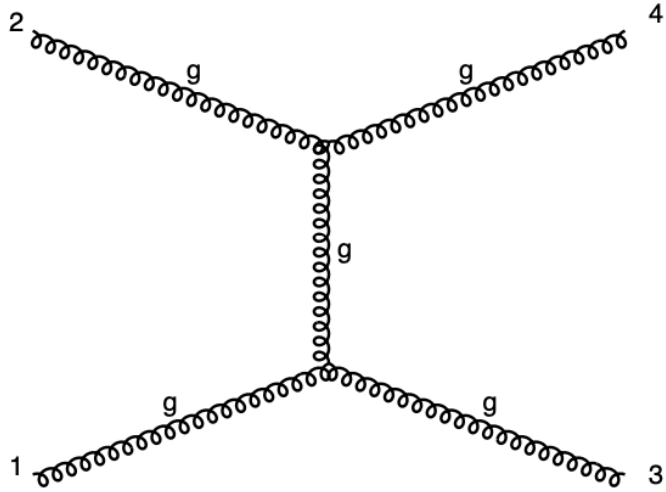


diagram 3

QCD=2, QED=0

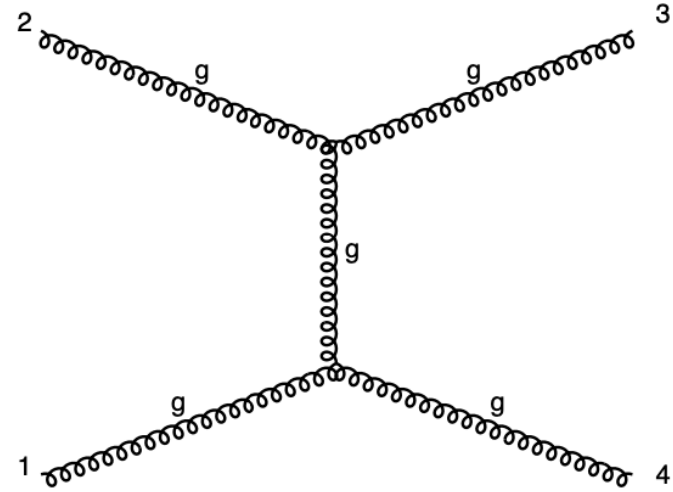
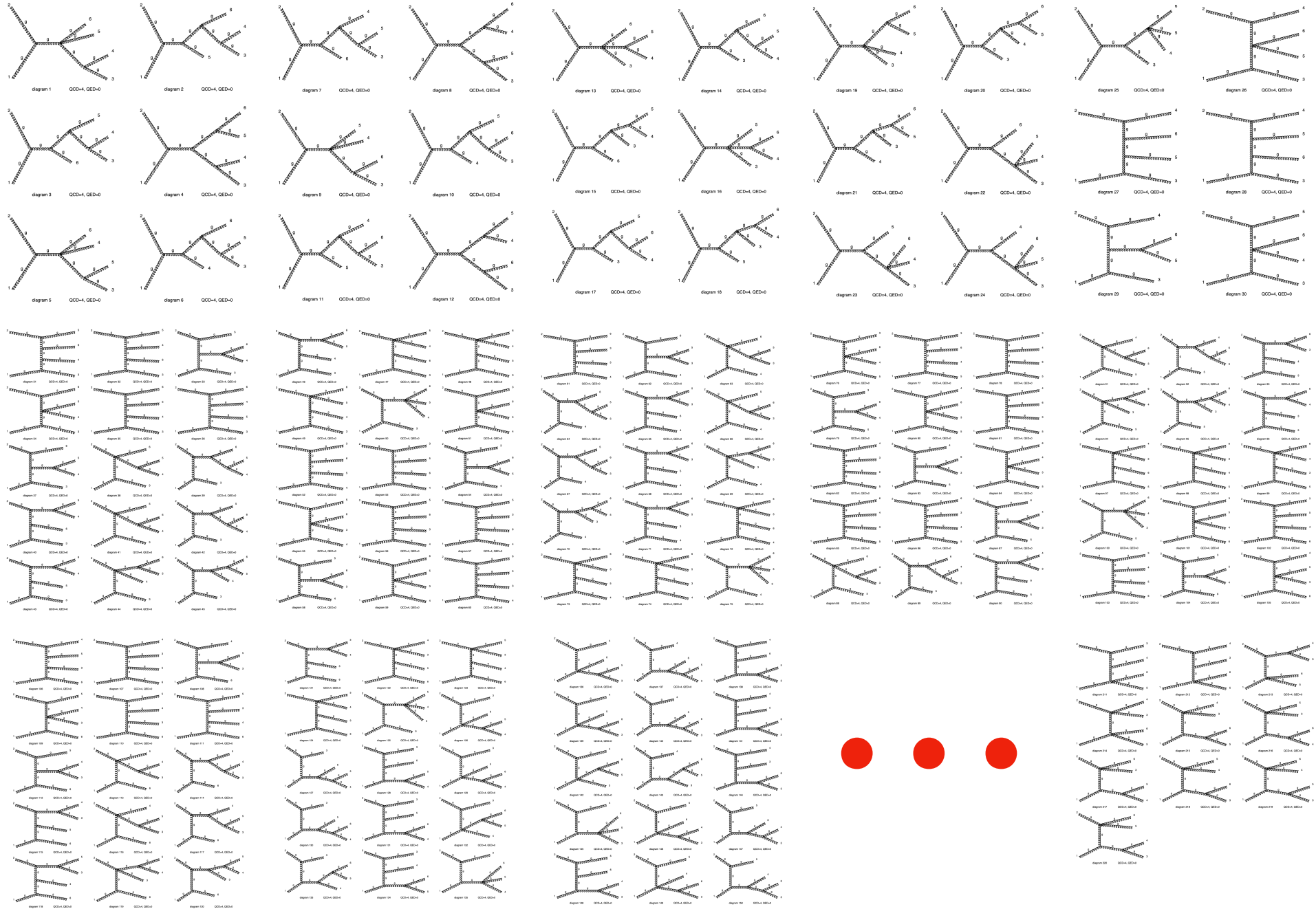


diagram 4

QCD=2, QED=0

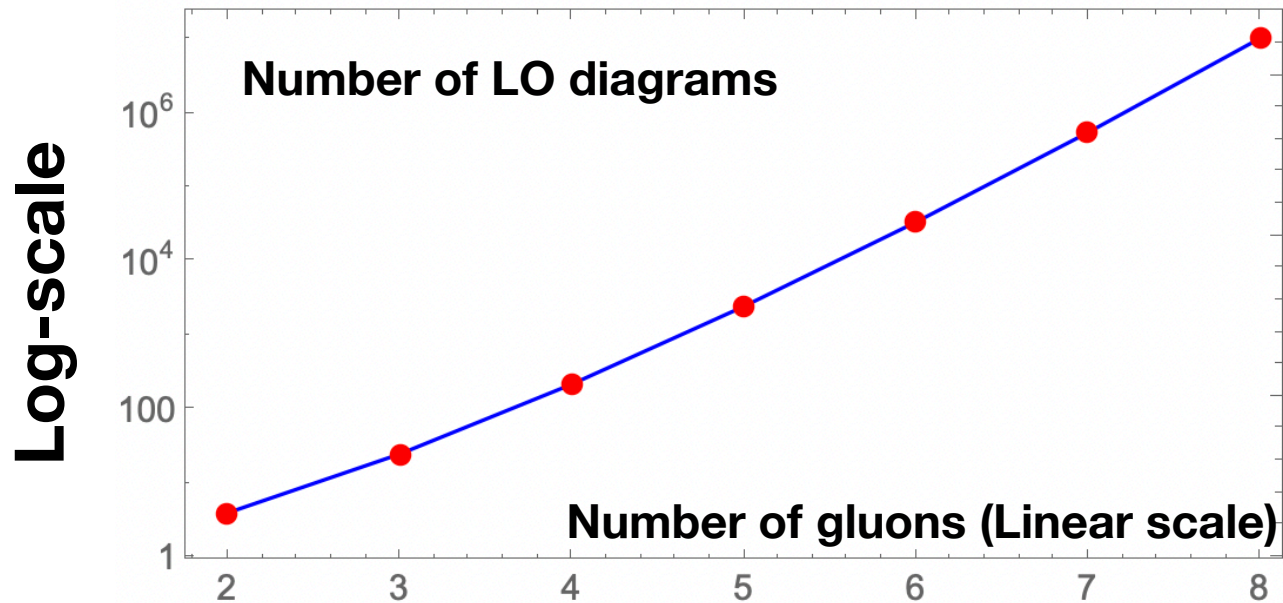
gg → gggg



Multiplicity !

- The production of multi-particles will have **HUGE number** of "feynman" diagrams.

	$gg \rightarrow 2g$	$gg \rightarrow 3g$	$gg \rightarrow 4g$	$gg \rightarrow 5g$	$gg \rightarrow 6g$	$gg \rightarrow 7g$	$gg \rightarrow 8g$
Number of LO diagrams	4	25	220	2,485	34,300	559,405	10,525,900

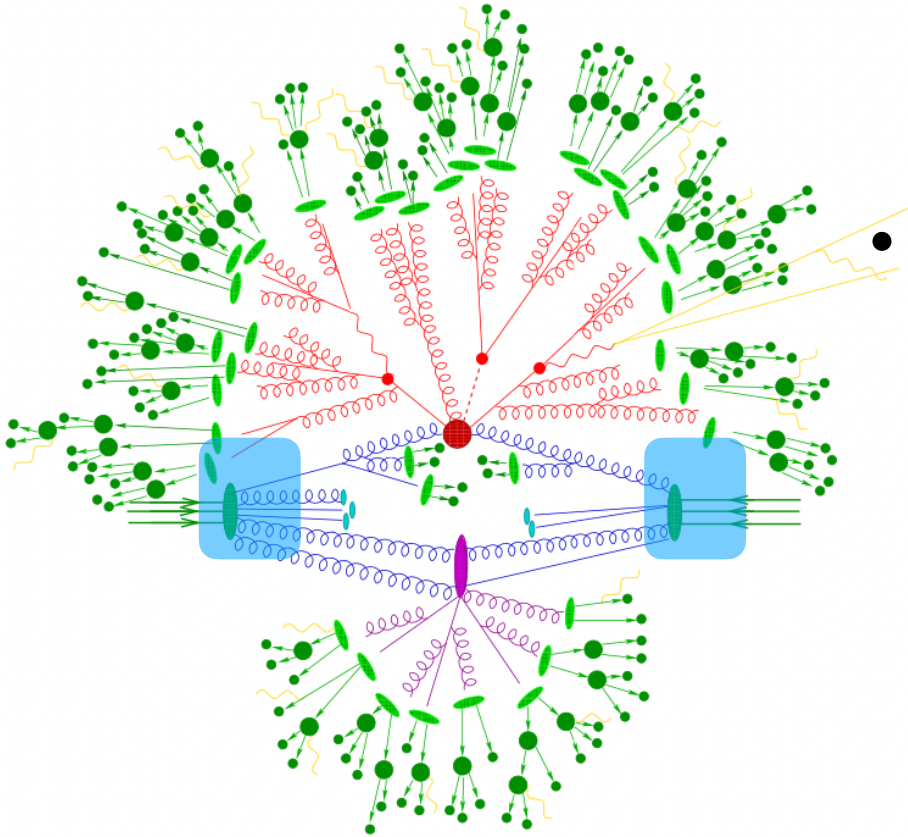


A Monte Carlo Generator

- Monte Carlo Generator is the essence of our understanding in various parts of "particle physics".
- Perturbative calculations, non-perturbative regions, Quantum Corrections.

Monte Carlo Simulation

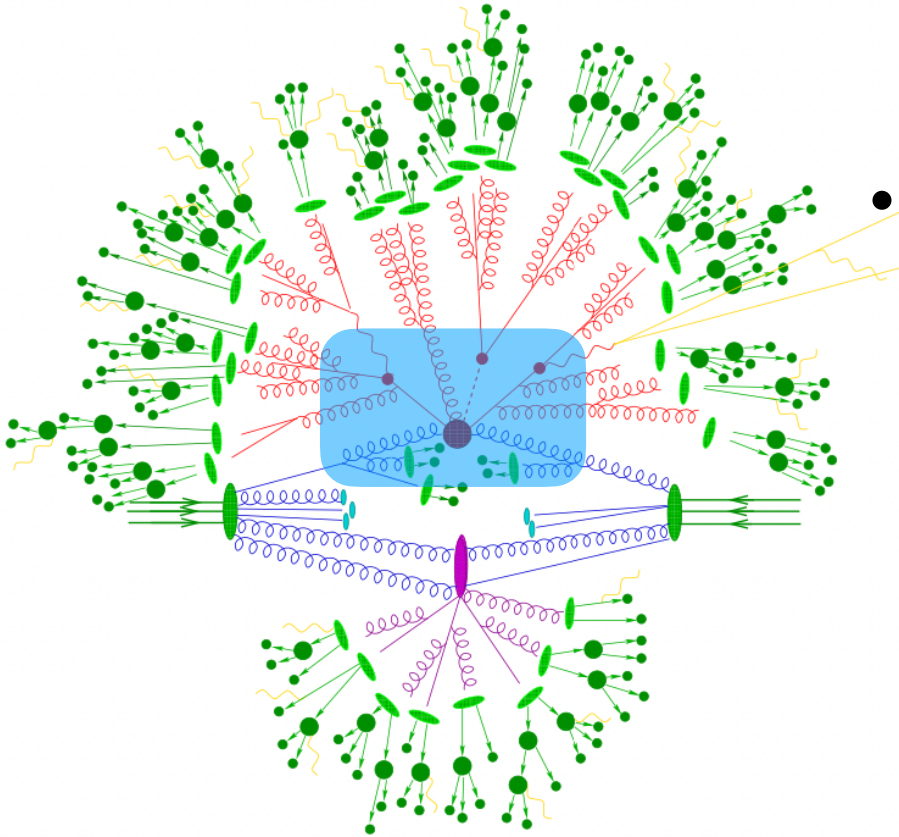
$$\mathcal{L}_{\text{theory}} \ni -\frac{1}{4}G_{\mu\nu}^a G^{a,\mu\nu} - \frac{1}{4}W_{\mu\nu}^i W^{i,\mu\nu} + \bar{q} \left(i\gamma^\mu D_\mu - m \right) q$$



- With $\mathcal{L}_{\text{theory}}$, we simulate a collision process with various Monte Carlo tools.
- **PDF : parton contributions**
(e.g. : quark/gluons in protons)

Monte Carlo Simulation

$$\mathcal{L}_{\text{theory}} \ni -\frac{1}{4}G_{\mu\nu}^a G^{a,\mu\nu} - \frac{1}{4}W_{\mu\nu}^i W^{i,\mu\nu} + \bar{q} \left(i\gamma^\mu D_\mu - m \right) q$$



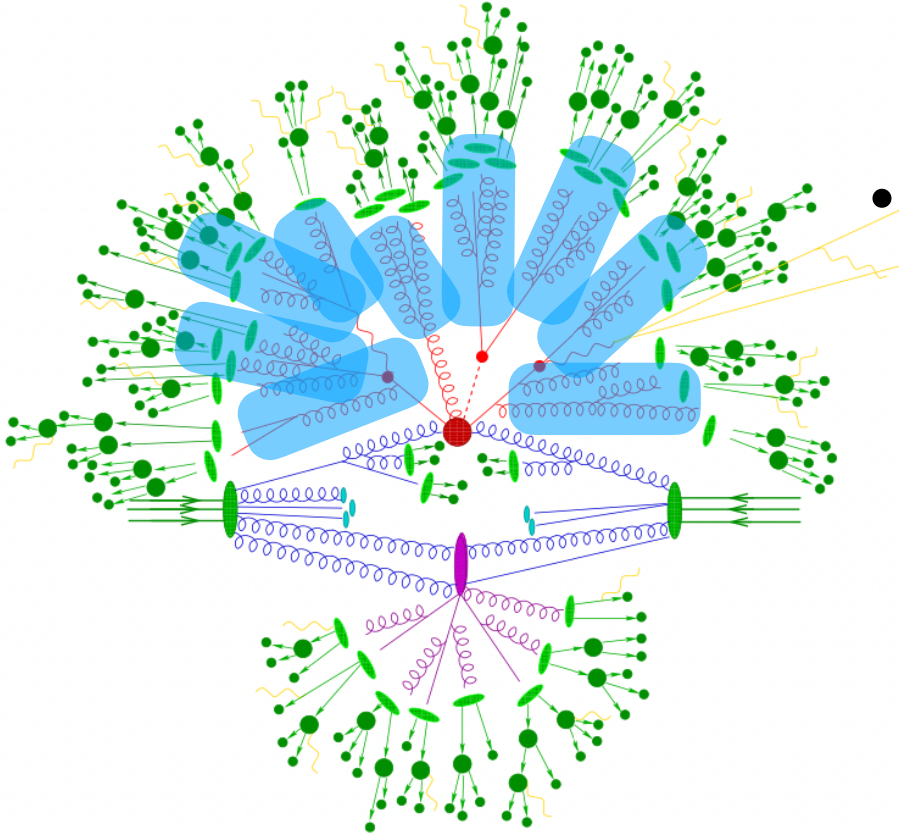
- With $\mathcal{L}_{\text{theory}}$, we simulate a collision process with various Monte Carlo tools.

- Hard process

(e.g: $gg \rightarrow t\bar{t} \rightarrow bW^+\bar{b}W^- \rightarrow b\bar{b}jjjj$)

Monte Carlo Simulation

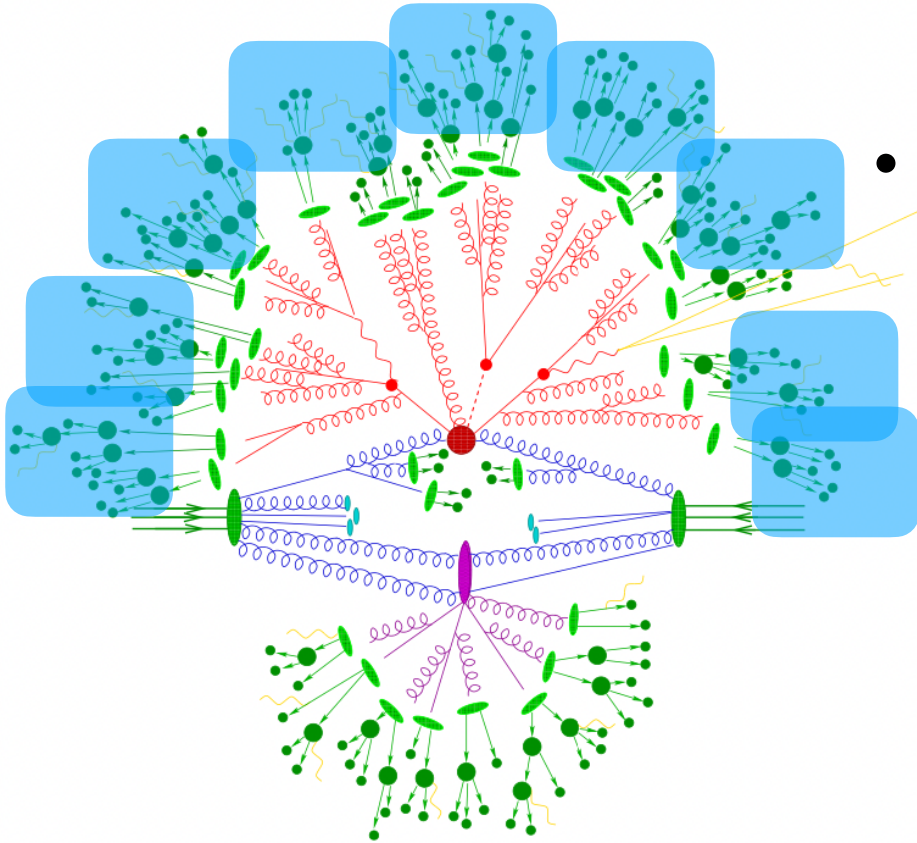
$$\mathcal{L}_{\text{theory}} \ni -\frac{1}{4}G_{\mu\nu}^a G^{a,\mu\nu} - \frac{1}{4}W_{\mu\nu}^i W^{i,\mu\nu} + \bar{q} \left(i\gamma^\mu D_\mu - m \right) q$$



- With $\mathcal{L}_{\text{theory}}$, we simulate a collision process with various Monte Carlo tools.

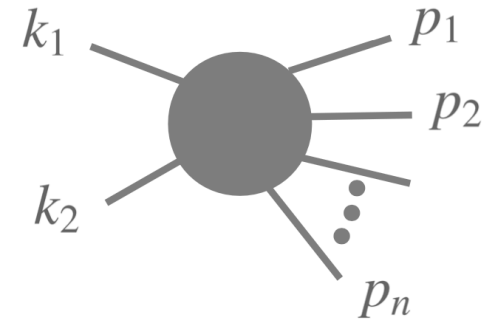
- **Parton Showering**
(soft radiations of charged particles)

Monte Carlo Simulation



- With $\mathcal{L}_{\text{theory}}$, we simulate a collision process with various Monte Carlo tools.
 - **Hadronization (approximation)**
(color dress-up : meson, hadron)
and **corresponding decays**

Our **First** target for



- $$\sigma = \frac{1}{2s} \int \prod_{i=1}^n \frac{d^3 p_i}{(2\pi)^3 2E_i} \delta \left(k_1 + k_2 - \sum_{i=1}^n p_i \right) |M_{fi}|^2 \theta_{\text{cut}}(p_1, \dots, p_n)$$

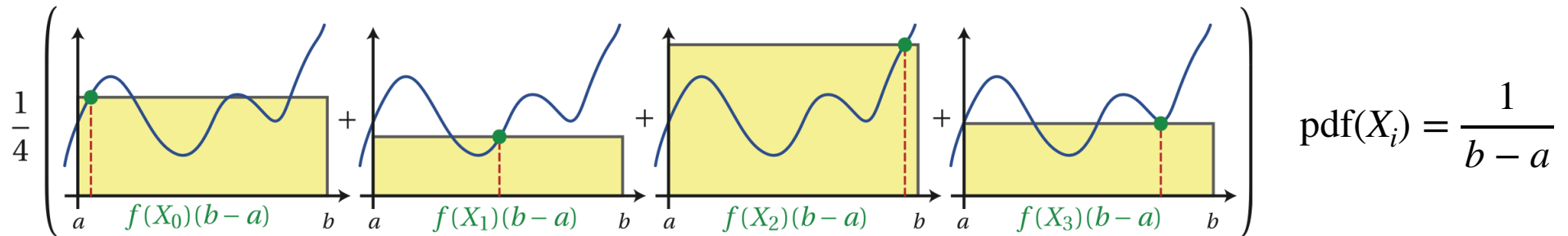
- For an observable $O(p_1, \dots, p_n)$, we need to calculate the differential distribution of

$$\frac{d\sigma}{dO} = \frac{1}{2s} \int \prod_{i=1}^n \frac{d^3 p_i}{(2\pi)^3 2E_i} \delta \left(k_1 + k_2 - \sum_{i=1}^n p_i \right) |M_{fi}|^2 \theta_{\text{cut}}(p_1, \dots, p_n) \delta(O - O(p_1, \dots, p_n))$$

(precise numerical) Integration
in high dimensional phase space

Monte Carlo with Importance sampling

- With random N samples according to a uniform Probability Distribution Function pdf(x) within an integral domain $[a, b]$



$$\langle F^N \rangle = \frac{1}{N} \sum_{i=0}^N \frac{f(X_i)}{\text{pdf}(X_i)} = (b-a) \frac{1}{N} \sum_{i=0}^N f(X_i)$$

$$\rightarrow E[\langle F^N \rangle] = (b-a) \frac{1}{N} \sum E[f(X_i)] = (b-a) \frac{1}{N} \sum \int_a^b f(X_i) \text{pdf}(x) dx = \int_a^b f(x) dx$$

$$\sigma[\langle F^N \rangle] = \frac{1}{\sqrt{N}} \sqrt{\sum_{i=0}^{N-1} \sigma^2 \left[\frac{f(X_i)}{\text{pdf}(X_i)} \right]}$$

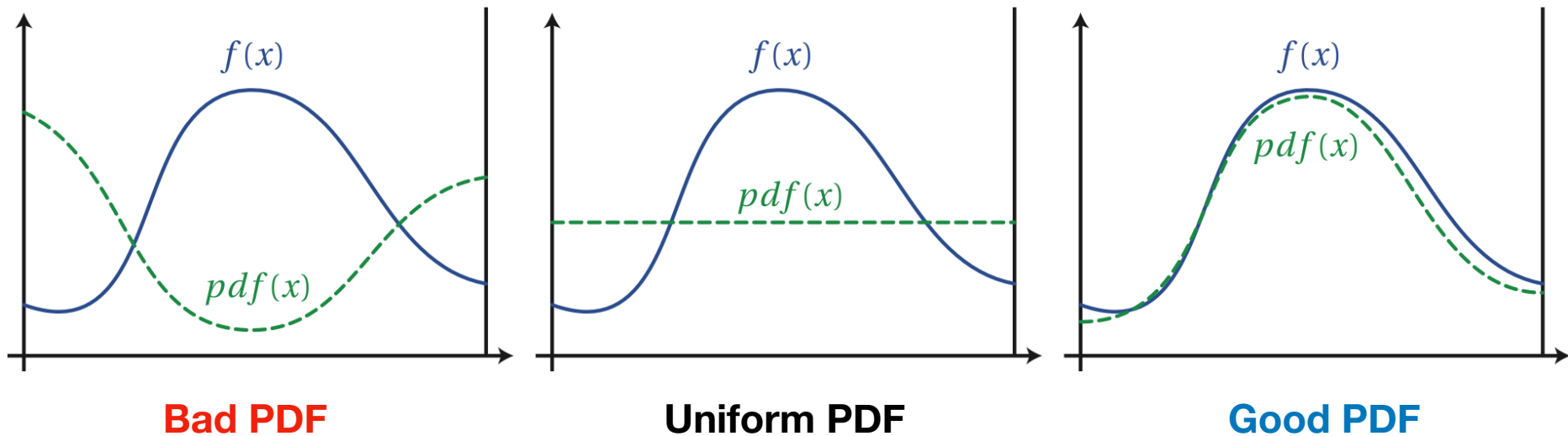
Random sampling

Importance sampling to reduce a variance

Importance sampling

- If we sample PDF $\propto f(x)$, we can reduce a variance

$$\sigma[\langle F^N \rangle] = \frac{1}{\sqrt{N}} \sqrt{\sum_{i=0}^{N-1} \sigma^2 \left[\frac{f(X_i)}{\text{pdf}(X_i)} \right]} \rightarrow \frac{1}{\sqrt{N}} \sqrt{\sum_{i=0}^{N-1} \sigma^2 \left[\frac{f(X_i)}{c f(X_i)} \right]} \approx \frac{1}{\sqrt{N}} \sqrt{\sum_{i=0}^{N-1} \sigma^2 \left[\frac{1}{c} \right]} \equiv \frac{1}{\sqrt{N}} \times 0$$



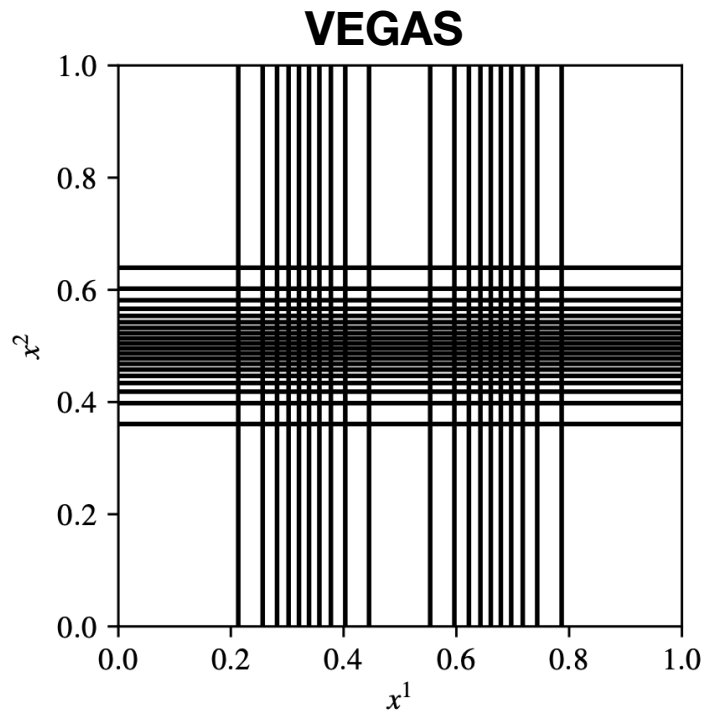
- When we don't know a function $f(x)$ at all, **how can we estimate a good PDF ?**

Traditional method...

- **Stratified Sampling:** Divide domain into sub-domains.

For example, if we divide the domain into N divisions,

$$\sigma \propto \frac{1}{N} \text{ instead of } \sigma \propto \frac{1}{\sqrt{N}}$$



- "Classic" VEGAS: **Adaptive** importance sampling, since 1977

Recently, there is an update, VEGAS+
J.Comput.Phys. 439 (2021) 110386

Neural Net (NN) as a good estimator

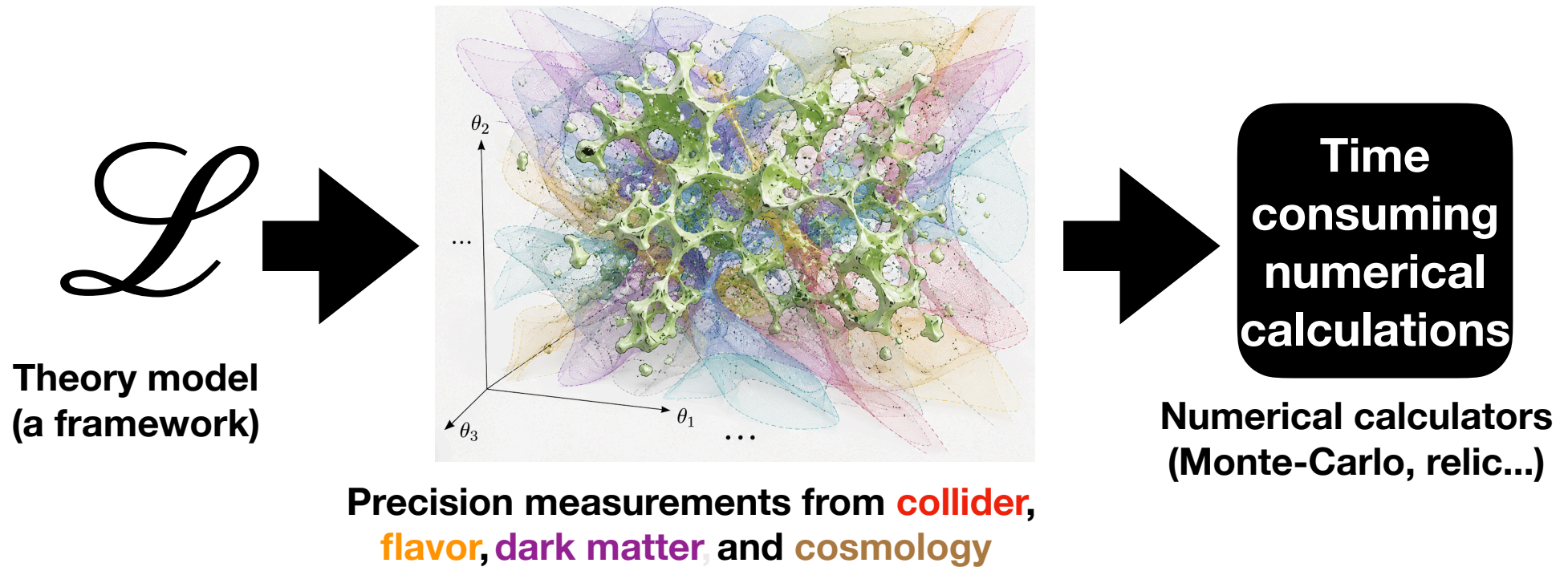
- Due to the universal approximation theorem, **NN serves as a bonafide function approximator.**
- Design a process where the accuracy of NN becomes proportional to our interests in sampled regions:
 - spend, relatively, more time to sample in **regions of interests**
 - enough time for low importance region

Importance sampling with Machine Learning

- In fact, we already solved a similar problem in our previous study [arXiv:2207.09959](https://arxiv.org/abs/2207.09959), (This project was a pilot project)

"Exploration of Parameter Spaces Assisted by Machine Learning"
(Computational Physics Communication, v293, 2023)
- Let me explain what we have done....

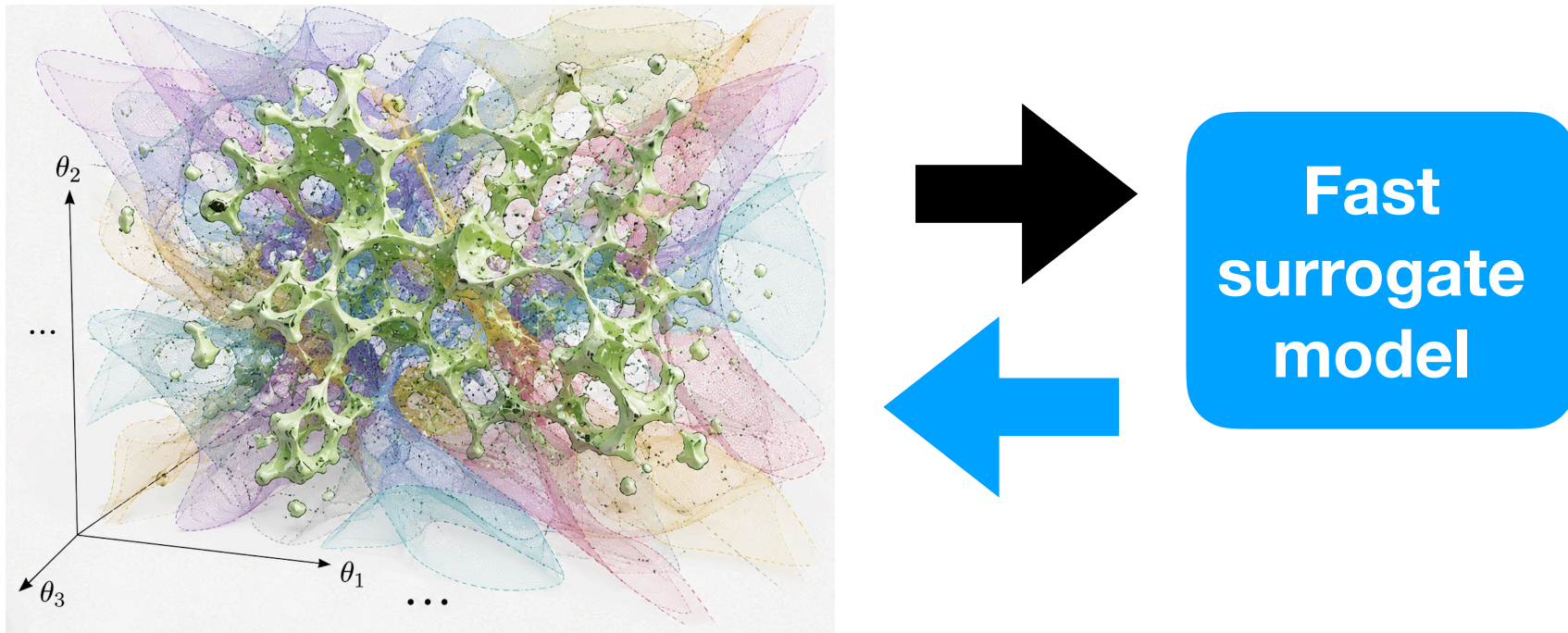
Conventional phenomenology



Highly constrained and irregular surviving parameter space

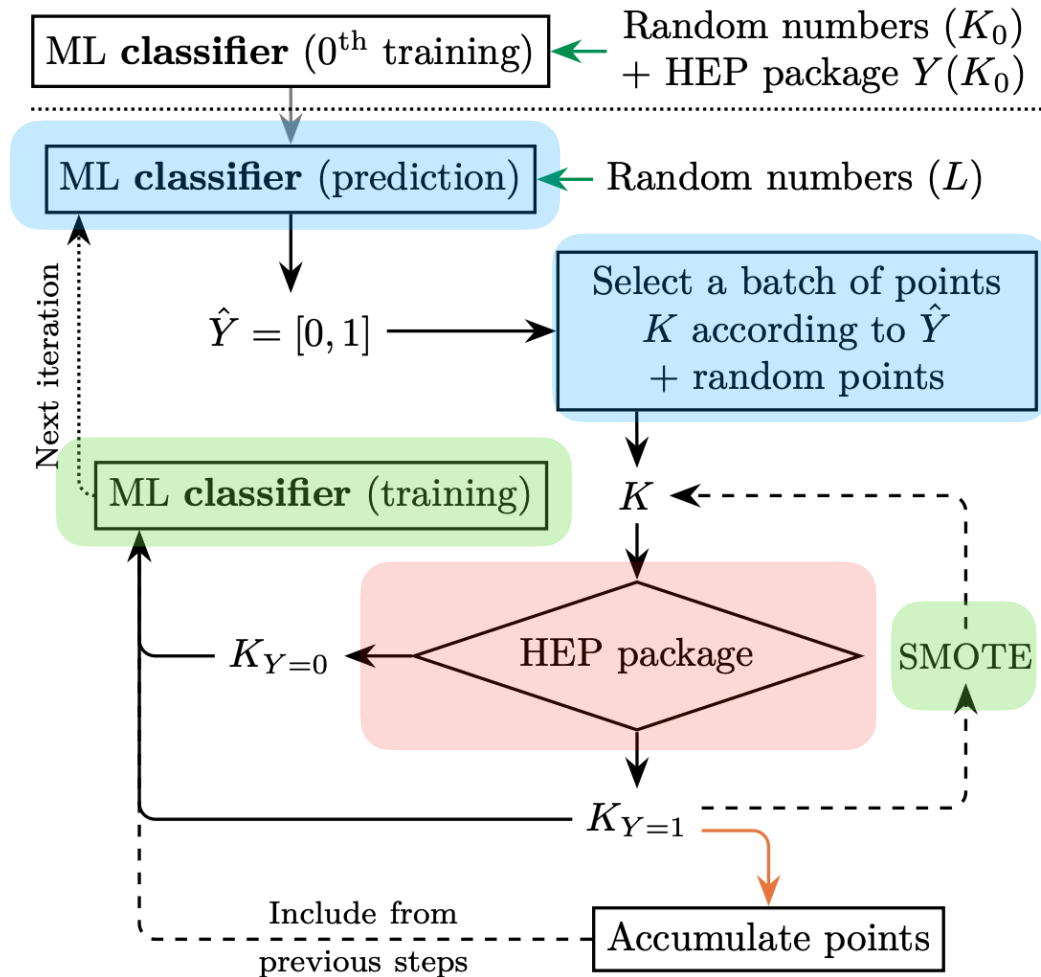
- Theoretical models often contain many free parameters.
- Precision measurements exclude large portions of the parameter space.
- The surviving parameter space is highly irregular, making brute-force scans increasingly inefficient.

AI assisted phenomenology



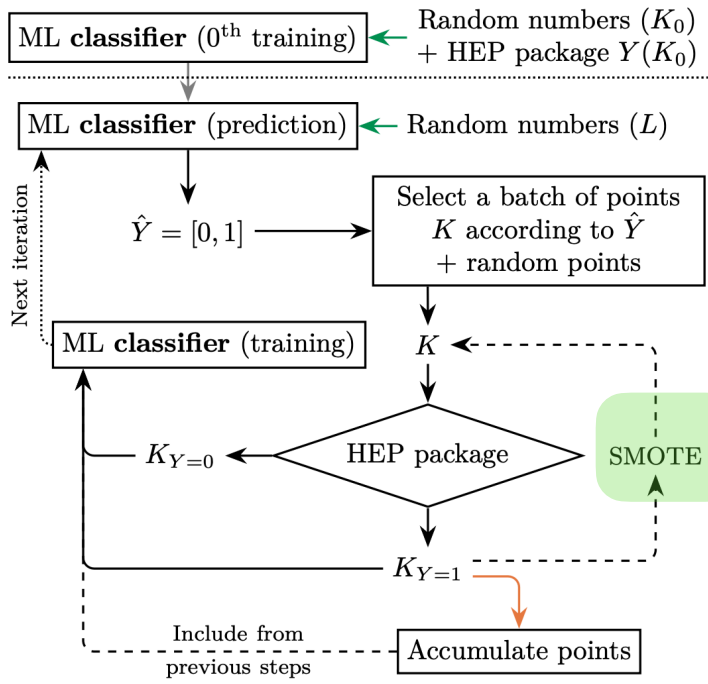
- We utilize AI to **approximate a heavy calculator** precisely
 - to reduce a time
- and to **suggest regions of interest**, not to waste a valuable time over unnecessary / uninteresting parameter regions

Classifier type ML



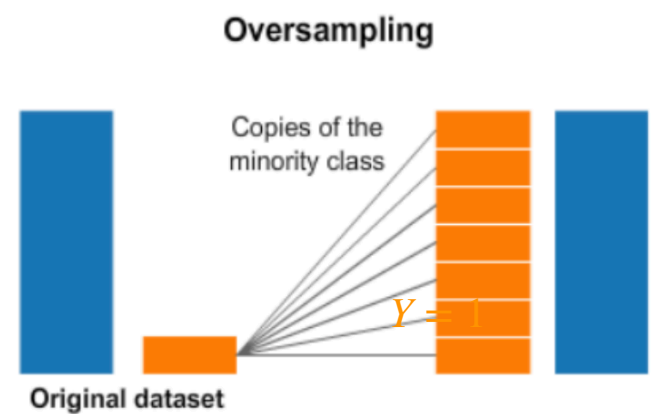
- **Generate initial random points**
 - Evaluate them with a HEP simulation package.
- **Train a classifier**
 - Learn whether a point is accepted $\hat{Y} = 1$ or rejected $\hat{Y} = 0$
- **Predict promising regions**
 - Apply the classifier to a large pool of unexplored points.
- **Select and evaluate new candidates**
 - Focus on points likely to satisfy the target conditions.
- **Update and repeat**
 - Add newly evaluated points to the dataset and retrain the classifier.

Data Augmentation using SMOTE



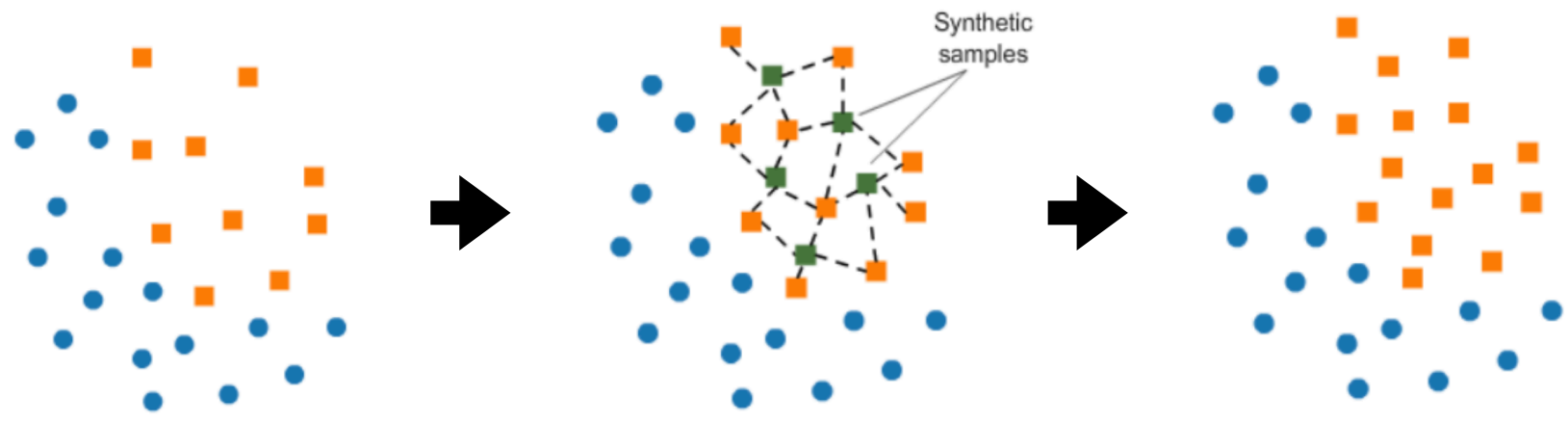
SMOTE (arXiv:1106.1813)

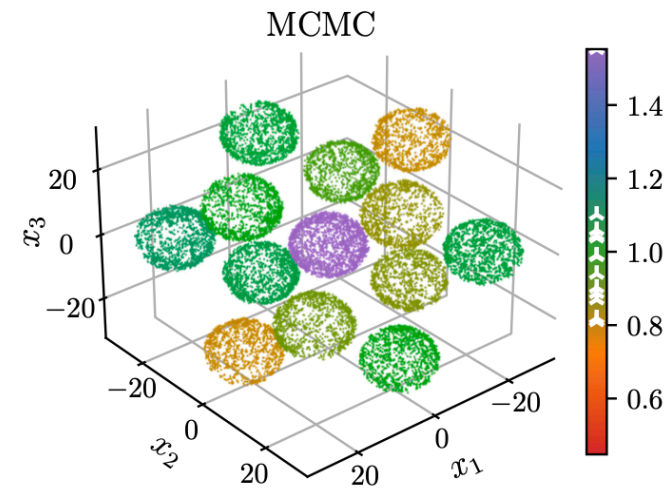
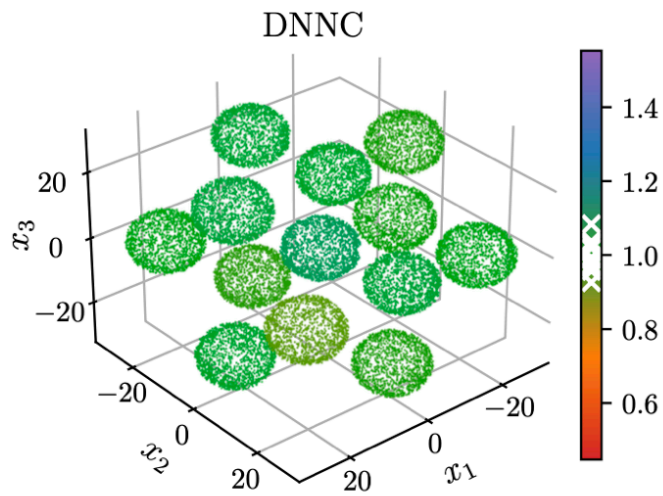
- **Synthetic Minority Oversampling Technique**



SMOTE generates artificial minority-class events by interpolating between nearby signal samples in feature space.

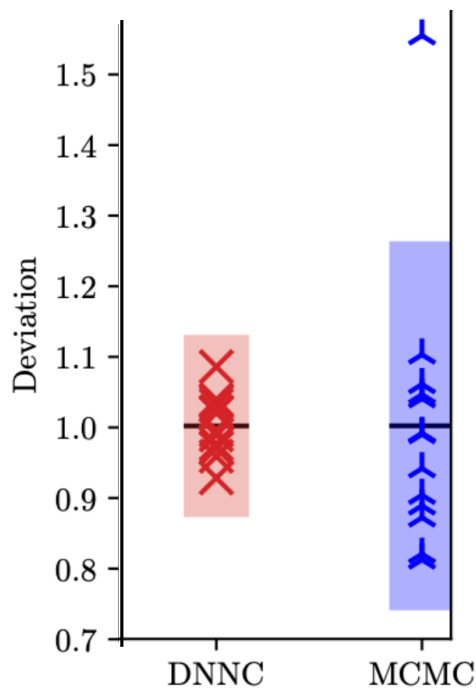
Generate synthetic minority-class samples using k-nearest neighbors





$$O_{3d} = \left[2 + \cos\left(\frac{x_1}{7}\right) \cos\left(\frac{x_2}{7}\right) \cos\left(\frac{x_3}{7}\right) \right]^5$$

$$\mathcal{L}_{3d} = \exp\left[-(O_{3d} - c_{3d})^2 / 2\sigma_{3d}^2\right]$$

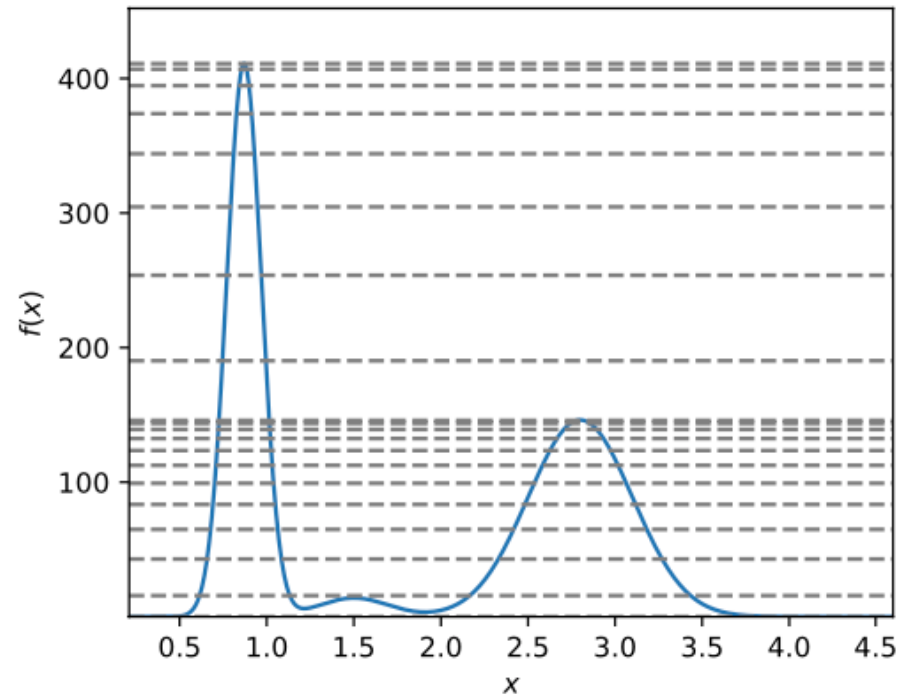
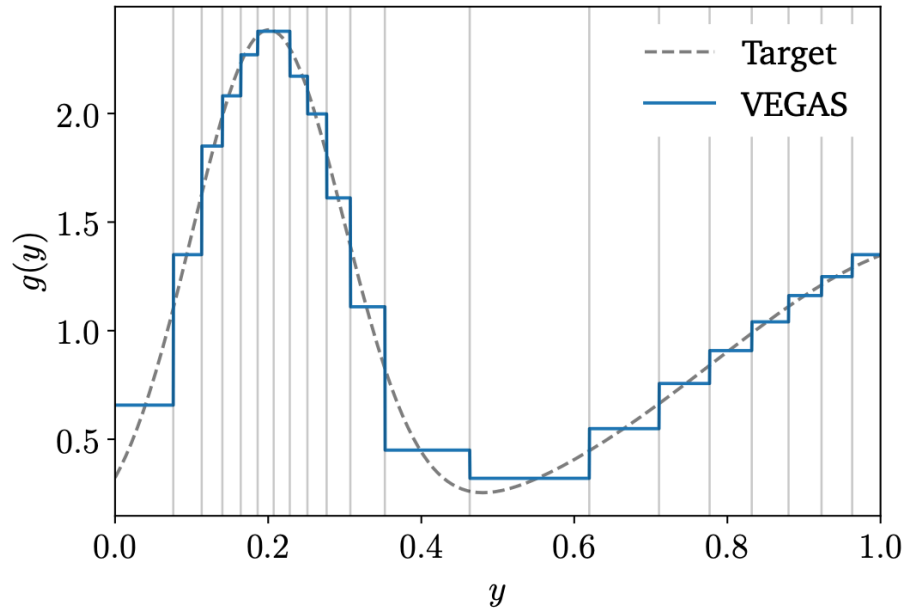


- Points are $\mathcal{L} > 0.9$ conditions.
- With $x_i \in [-10\pi, 10\pi]$, there are 13 cell.
- The "**deviation**" is the ratio of **a population in each "cell"** over an average population

**Utilizing our ML algorithm
for an importance sampling
in an integration**

Two integration methods

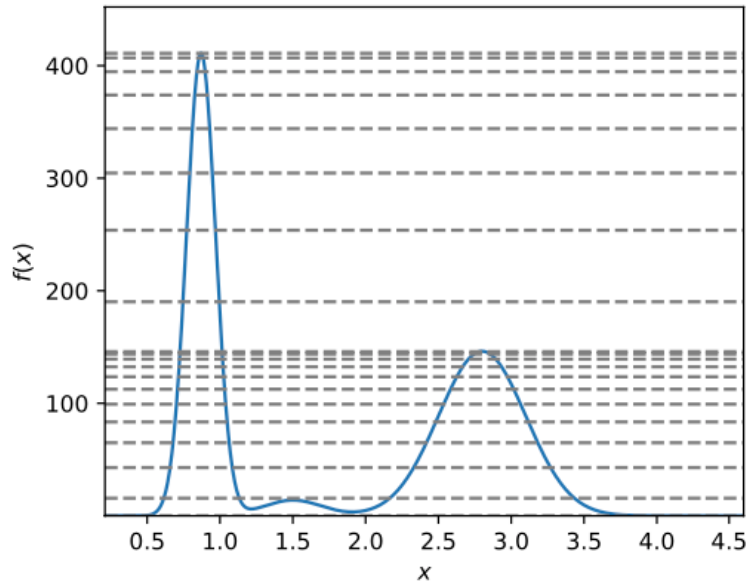
from MadNIS (Theo Heimel et.al. arXiv:2311.01548)



- **Riemann** Integration.
- **Lebesgue** Integration
- **Lebesgue integration provides a natural framework for importance sampling.**

- A classical example: $f(x) = \begin{cases} 1 & \text{if } x \in P \\ 0 & \text{if } x \in Q \end{cases}$

Our approach: Lebesgue



- Divide the space of integrand (**classes**)

$$\Phi_j = \{ \vec{x} \mid l_j < f(\vec{x}) \leq l_{j+1} \}$$

- The integral : $I_{\Phi} [f(\vec{x})] = \int_{\Phi} d^d x f(\vec{x}) = \sum_{j=1}^n \int_{\Phi_j} d^d x f(\vec{x}) = \sum_{j=1}^n V_{\Phi_j} \langle f \rangle_{\Phi_j}$

V_{Φ_j} : Volume of Φ_j .

- We recast the **problem of integration** → **classification problem**

example

- $\infty - \infty = \text{finite}$: We are testing "fine-tuning" function of

$$f_1(x_1, x_2) = g(x_1; 5, 2)g(x_2; 0, 2)$$

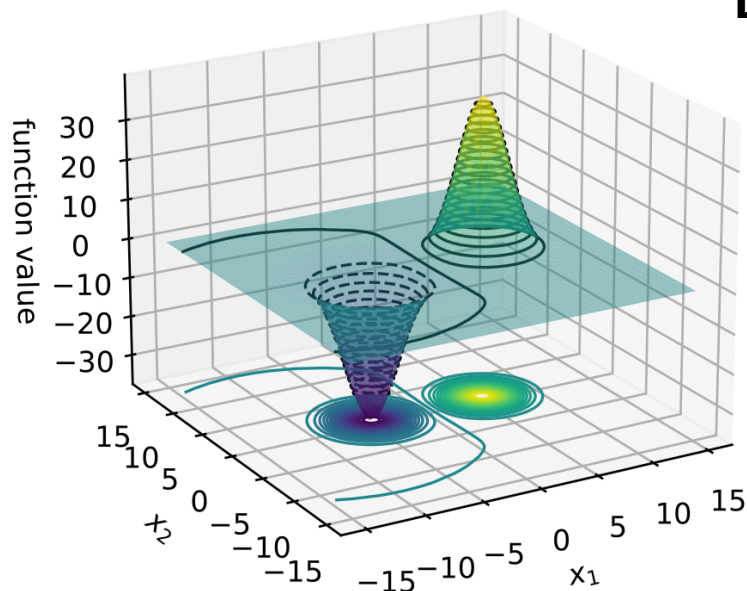
$$f_2(x_1, x_2) = g(x_1; -5, 2.1)g(x_2; 0, 2.1)$$

$$f_3(x_1, x_2) = g(x_1; 0, 3)g(x_2; 0, 3)$$

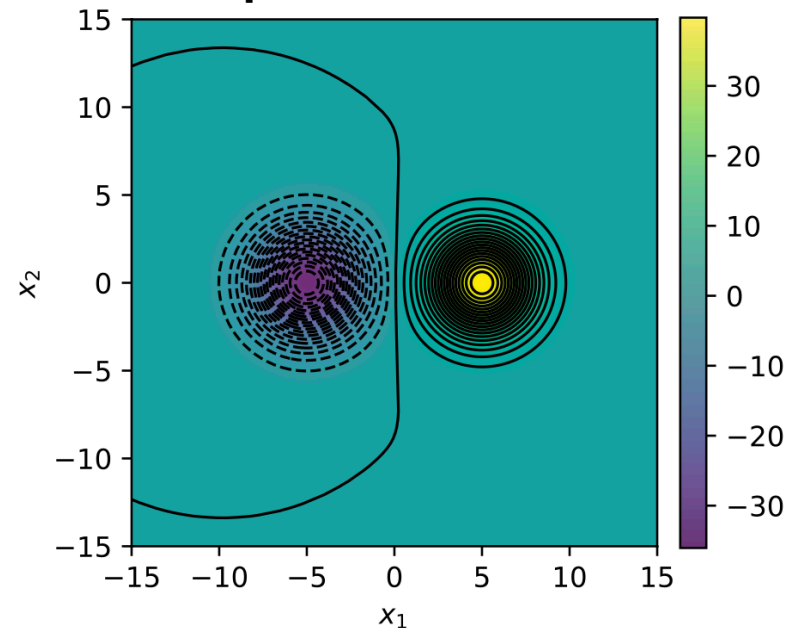
$$\text{with } g(x; m, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x-m)^2}{2\sigma^2}\right]$$

$$f(x_1, x_2) = 1000 [f_1(x_1, x_2) - f_2(x_1, x_2)] + f_3(x_1, x_2)$$

$$\int f(\vec{x}) dx dy \simeq 1$$

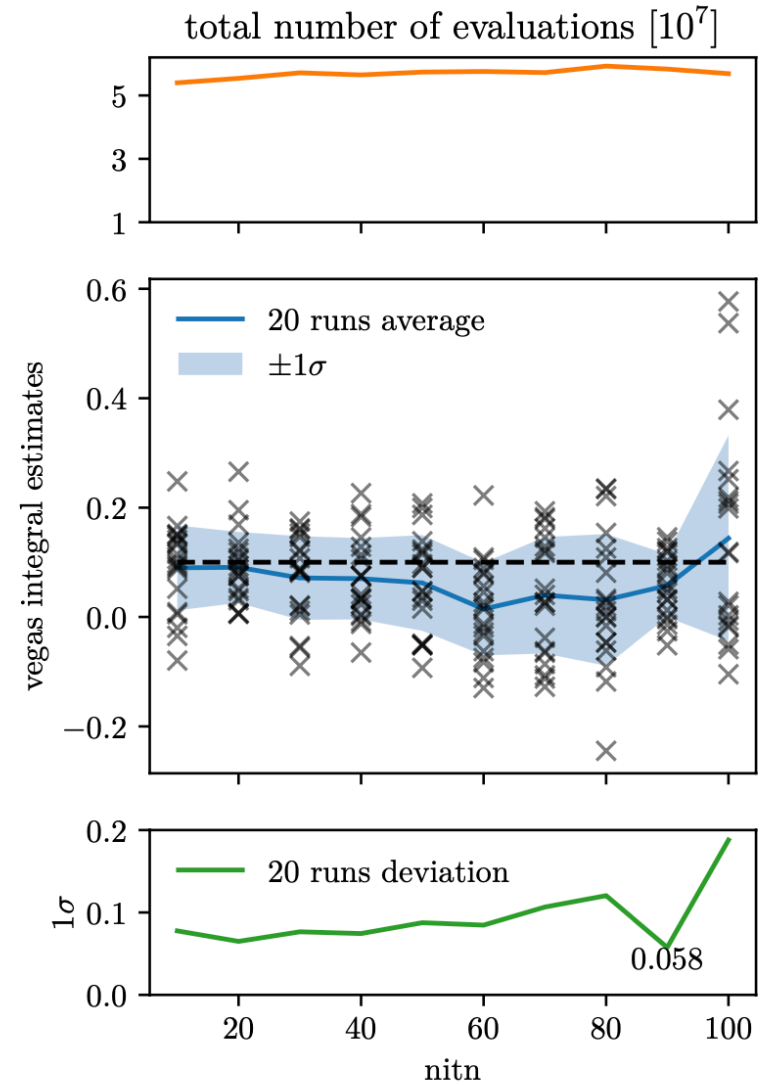
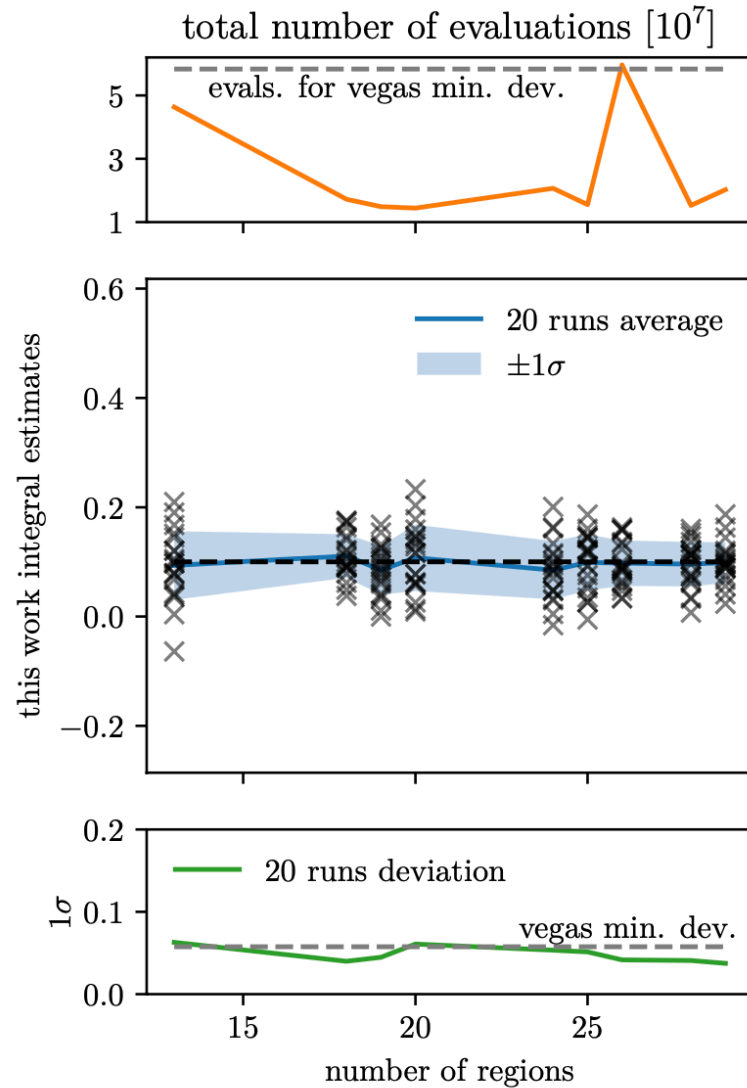


Divisions for equal "absolute" contributions



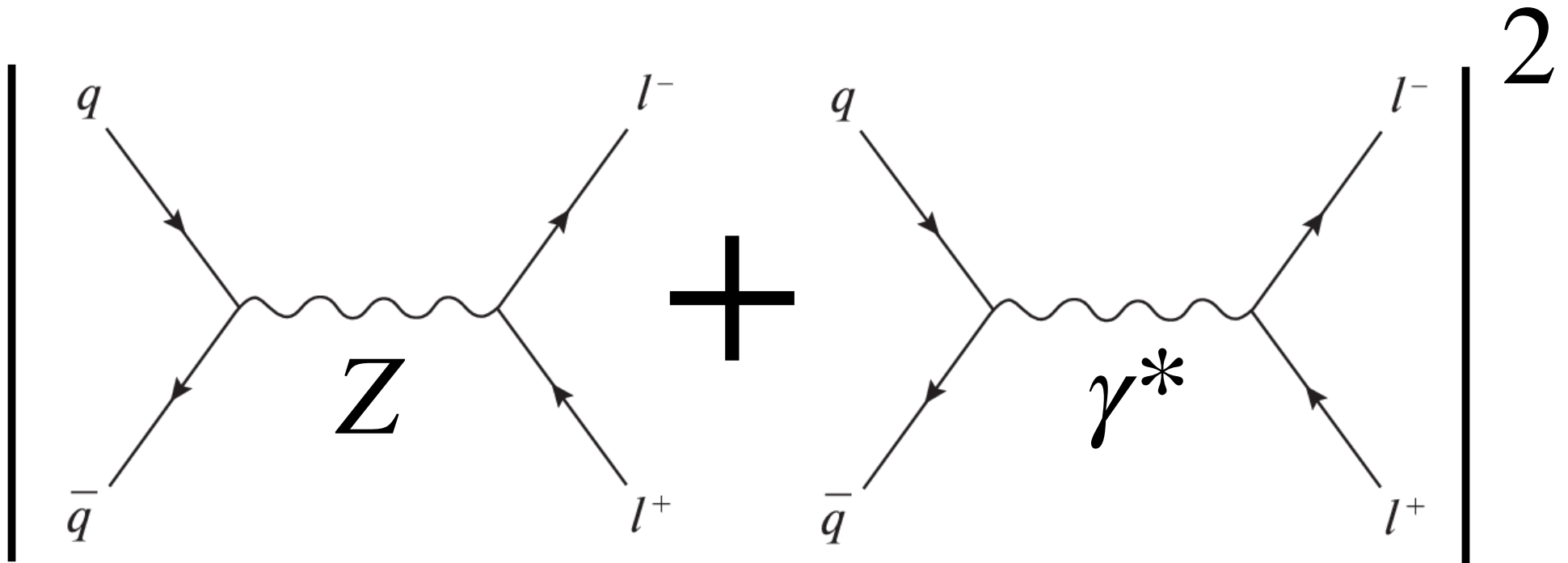
$$G(\vec{x}; \vec{\mu}, \sigma) = \prod_{j=1}^7 g(x_j; \mu_j, \sigma)$$

$$f_{7D}(\vec{x}) = 100 \times [G(\vec{x}; \vec{\mu}_+, \sigma_+) - G(\vec{x}; \vec{\mu}_-, \sigma_-)] + 0.1 \times G(\vec{x}; \vec{0}, \sigma_0)$$

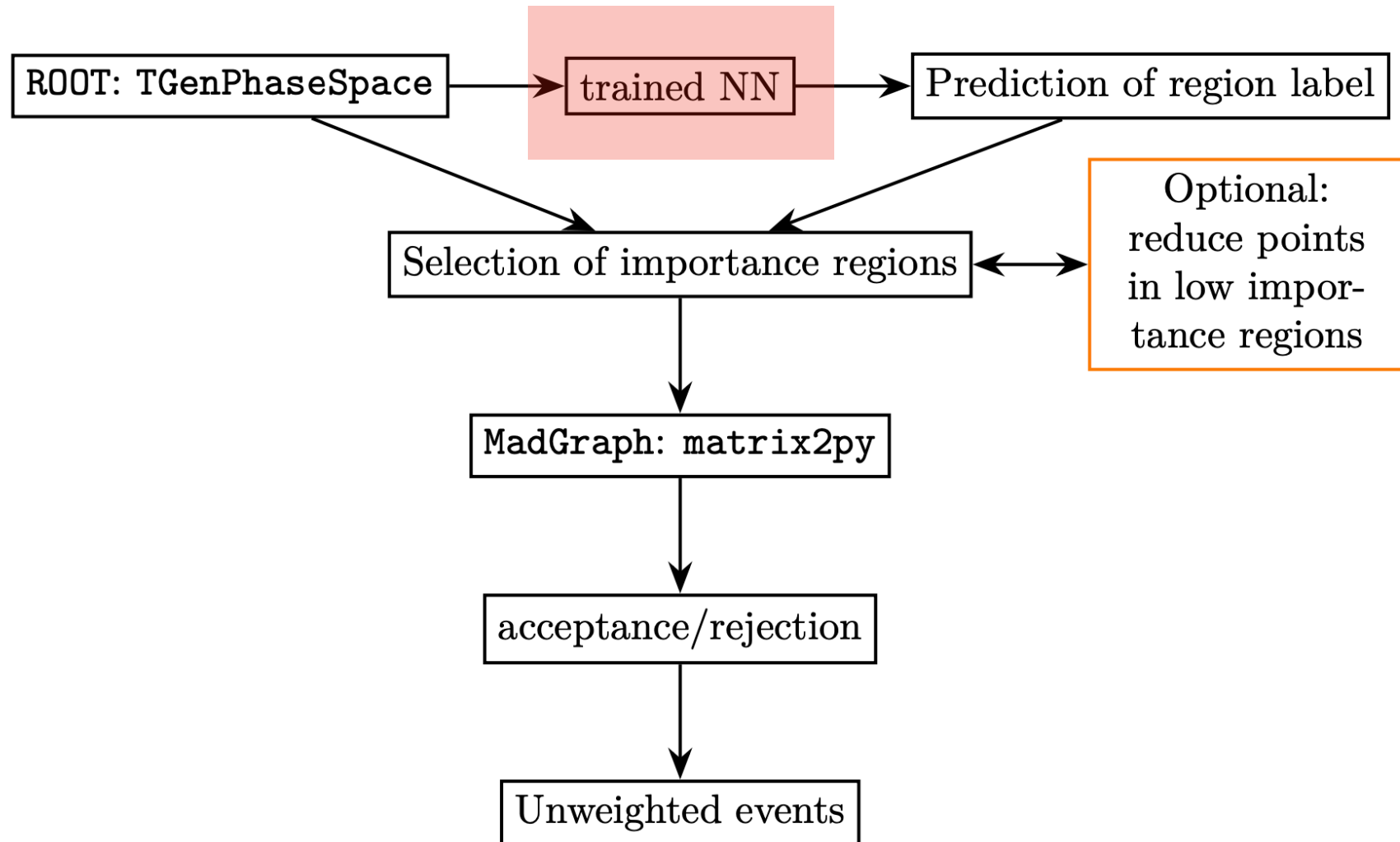


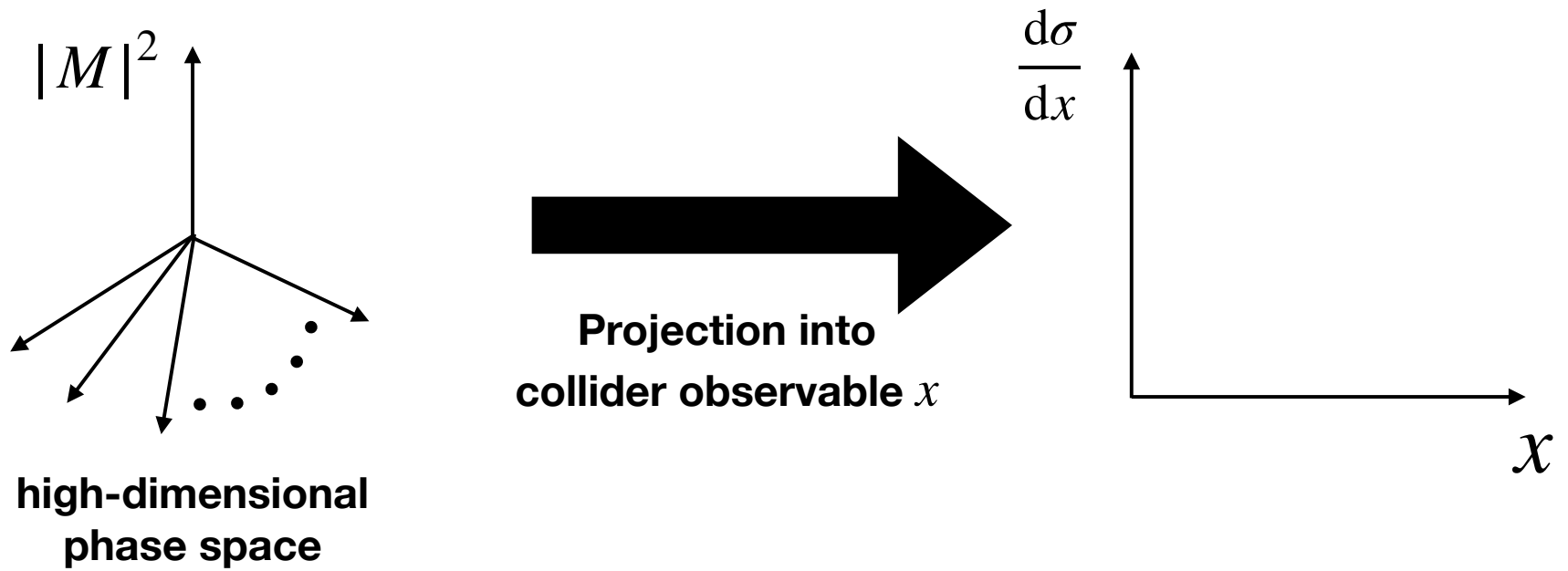
The Physics

$2 \rightarrow 2$ process with interference

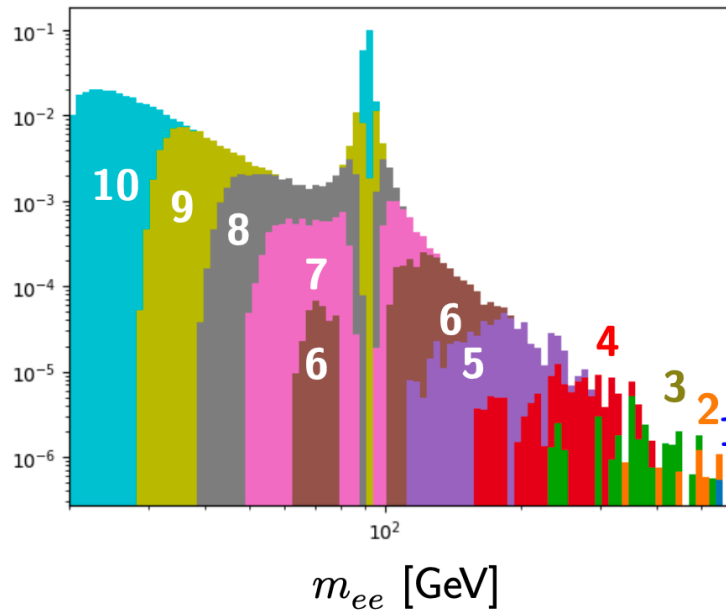


Generating MC samples with NN



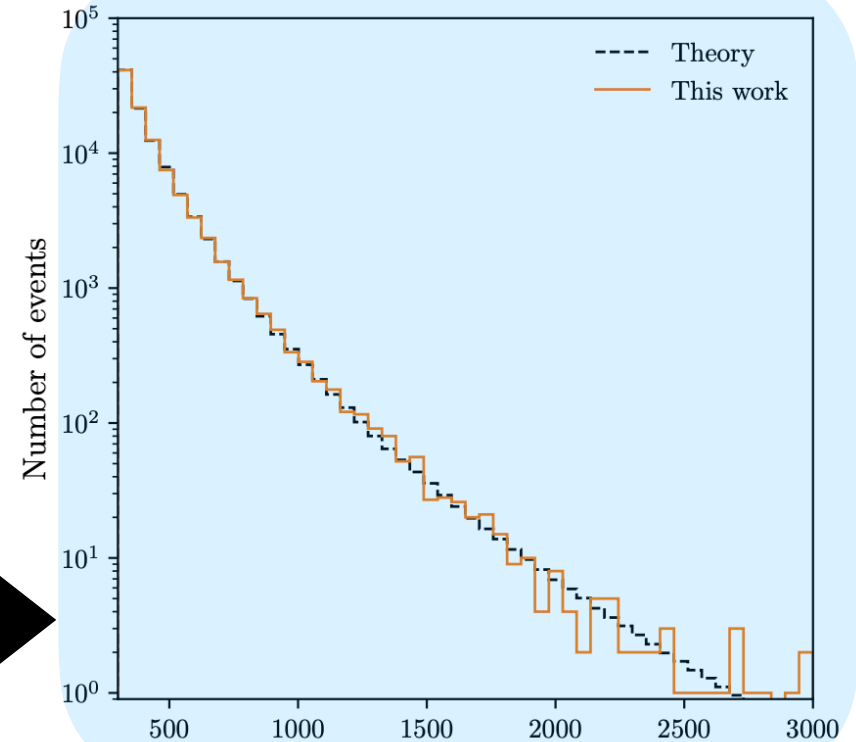
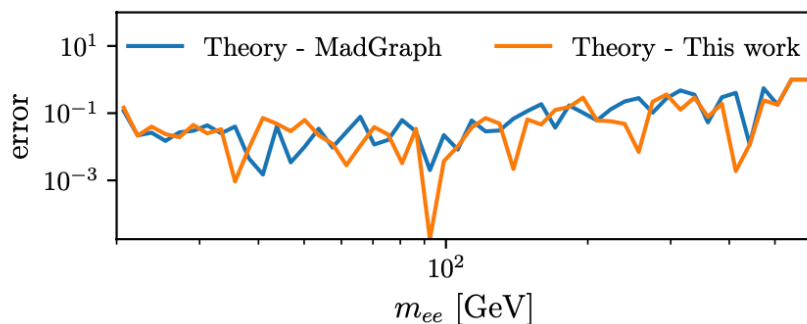
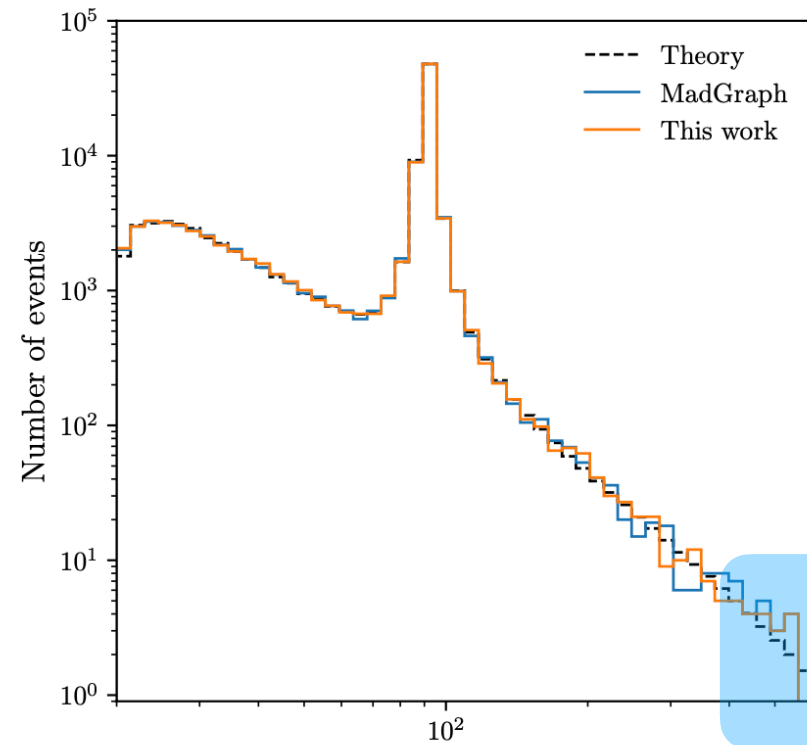


e^-e^+ invariant mass projection



- ▶ Sample each region until enough events are accumulated.
- NN can tell which regions points belong to.**
- ▶ Select points using correct result.

Sample as long as we want



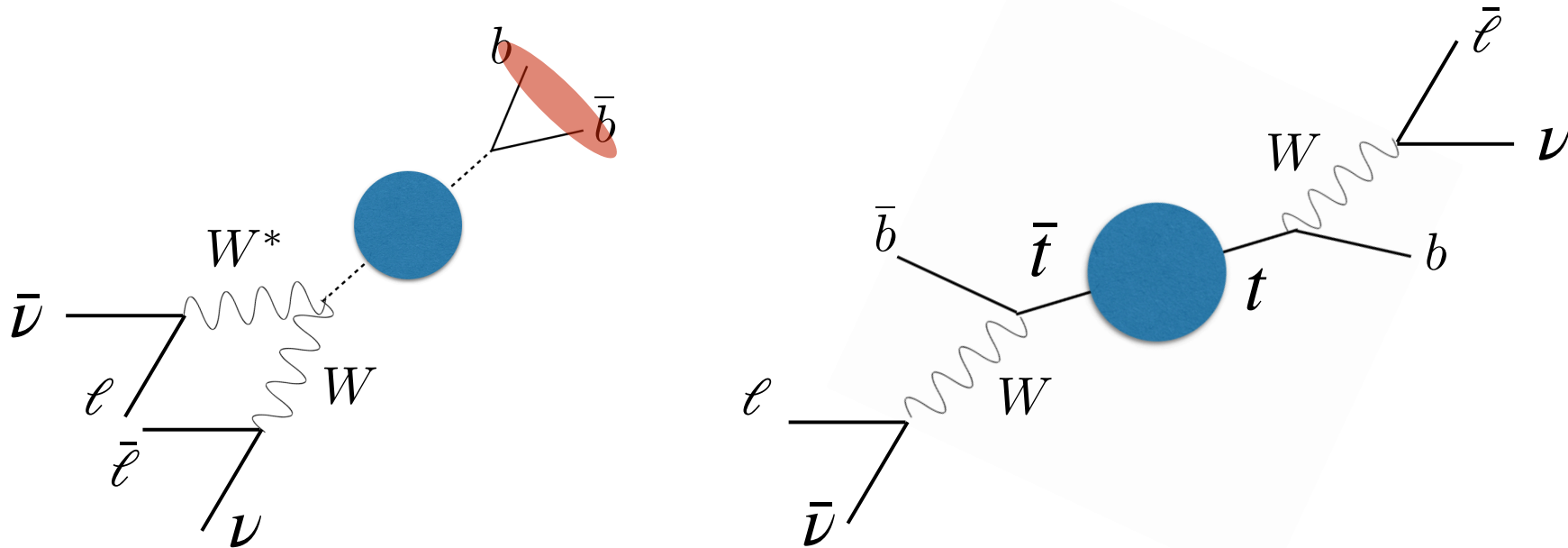
- We can zoom into "rare events"

Based on the assumption: With good enough Monte Carlo

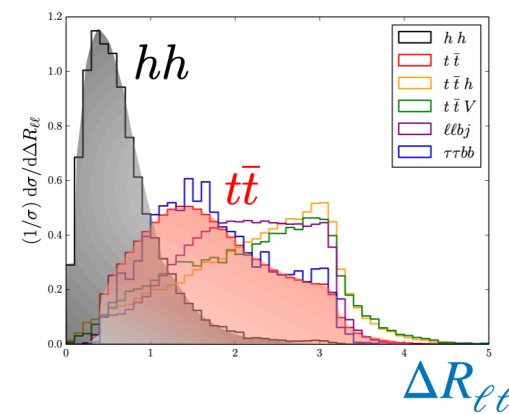
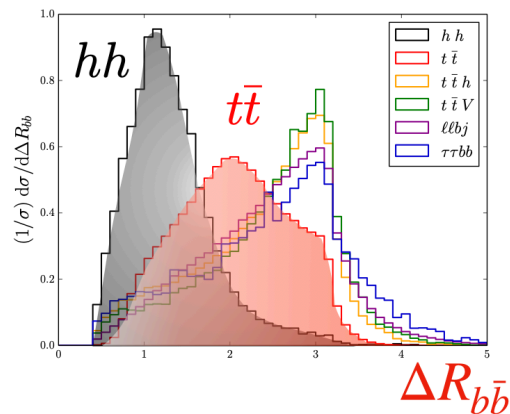
- I will explain how one can do the "supervised" ML for the LHC analyses.
- Of course, we need to have an efficient (Not so much data-hungry) ML

-
- Parton level information: Kinematics
 - Parton shower and hadronization: Gauge "charge"
 - How can we maximize the combination of two different types of information?

Parton level information



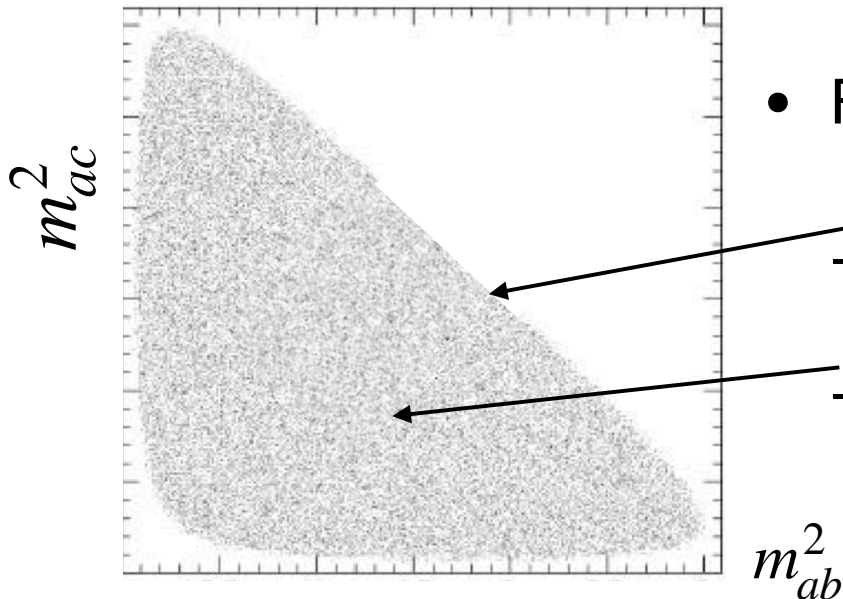
- **Kinematic variables** to utilize a **different phase-space** structures (signal, v.s. backgrounds)



Kinematics: Global information

- Differences in kinematics are from "high P_T " region, i.e. reconstructed level
 - Telling us about the structure of "Feynman-diagram"
(Event-topology, Mass spectrum)
- We can further utilize $|\mathcal{M}|^2$ differences (**Density** bounded by phase-space)

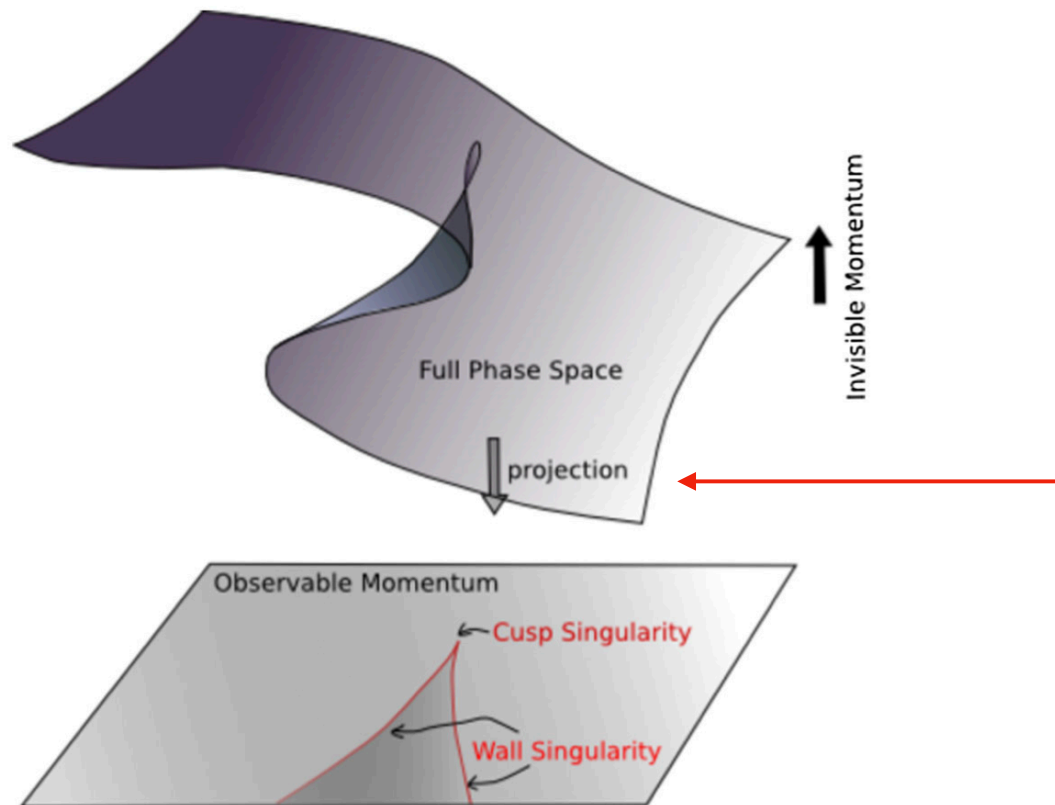
Classic example: Dalitz plot



- For example, $X \rightarrow a, b, c$

- **Boundary:** Structure of $1 \rightarrow 3$ phase space
- **Density:** information on **spin**

- Constructing an "observable" from a multi-dimensional phase space is **non-trivial**. (Especially when there is missing information)

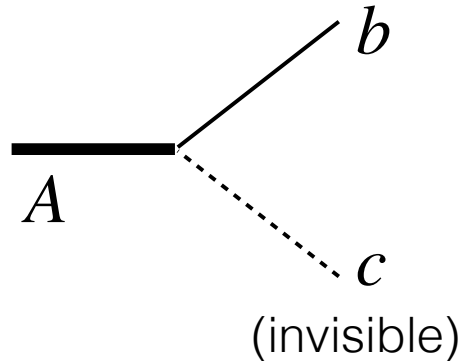


- Finding a suitable projection to maximize the **feature** of a full phase-space

Ian-Woo Kim 2010

Feature Engineering

- **Kinematic variables** to utilize a **different phase-space** structures (signal, v.s. backgrounds)



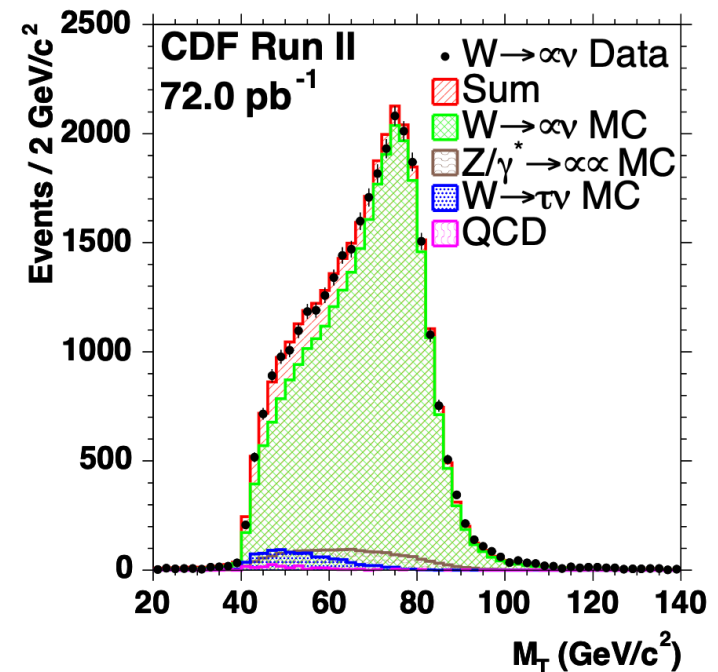
$$\theta = \{m_A\} \longrightarrow X = \{p_b^\mu, p_c^T\}$$

3: 3-Momentum from visible particle

2: Transverse Momentum from imbalanced situation

$$\dim(X) = 3 + 2 \rightarrow \dim(V) = 1$$

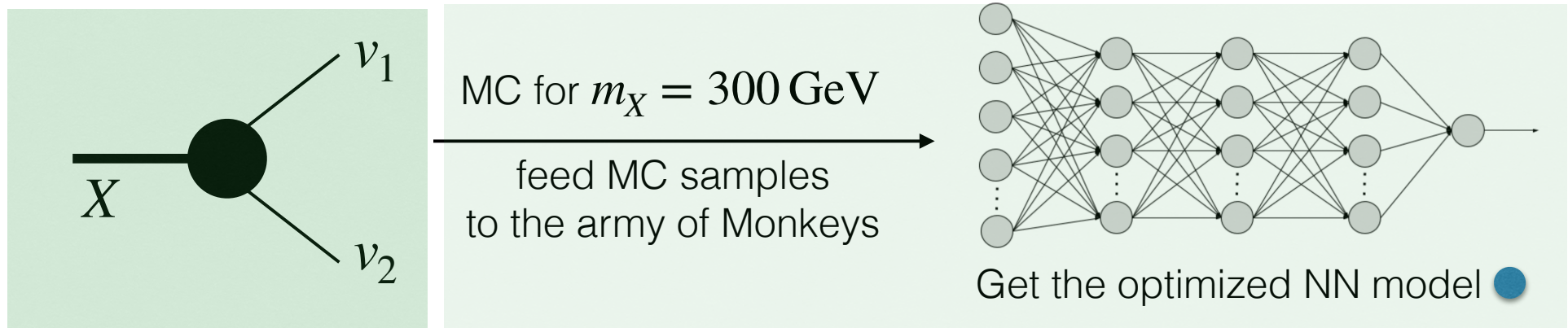
- **A human-engineered feature variable, M_T** which estimates m_A with an endpoint of its distribution
(highly singular behavior due to its Jacobian peak)



**Can AI automatically construct
an optimal observable?**

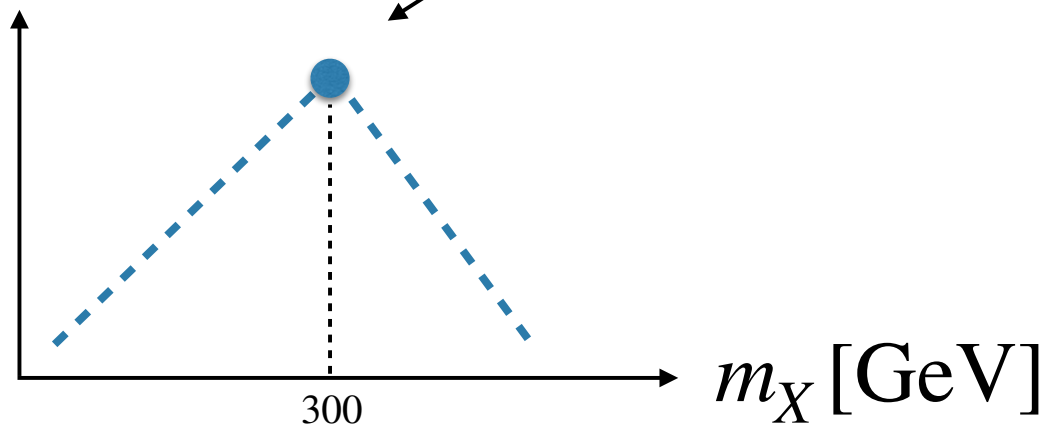
Example: Bump hunting

- **Conventional** supervised ML,

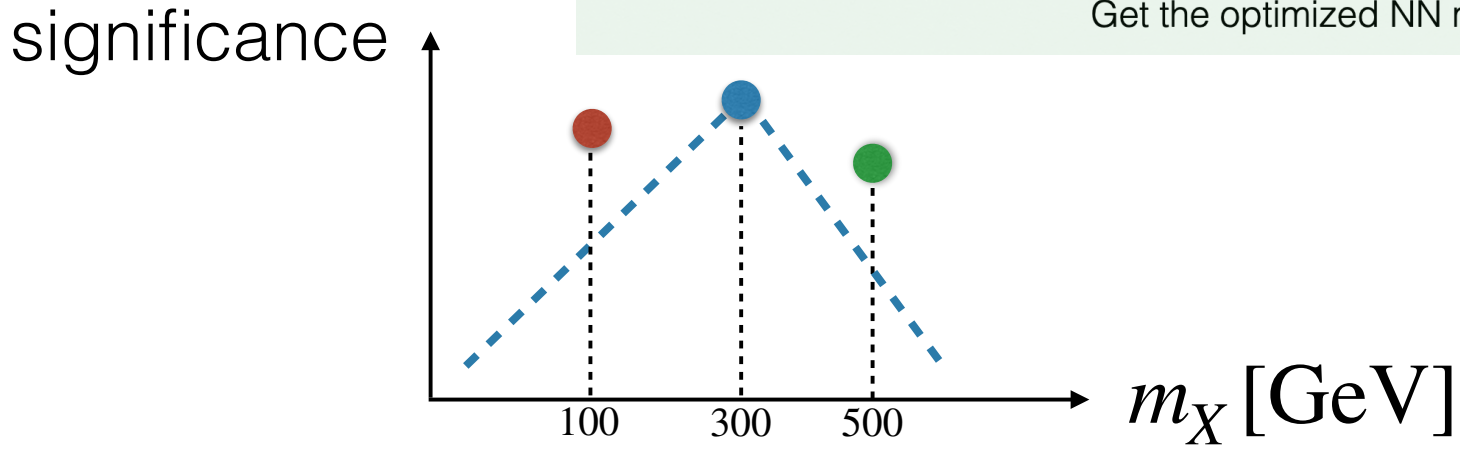
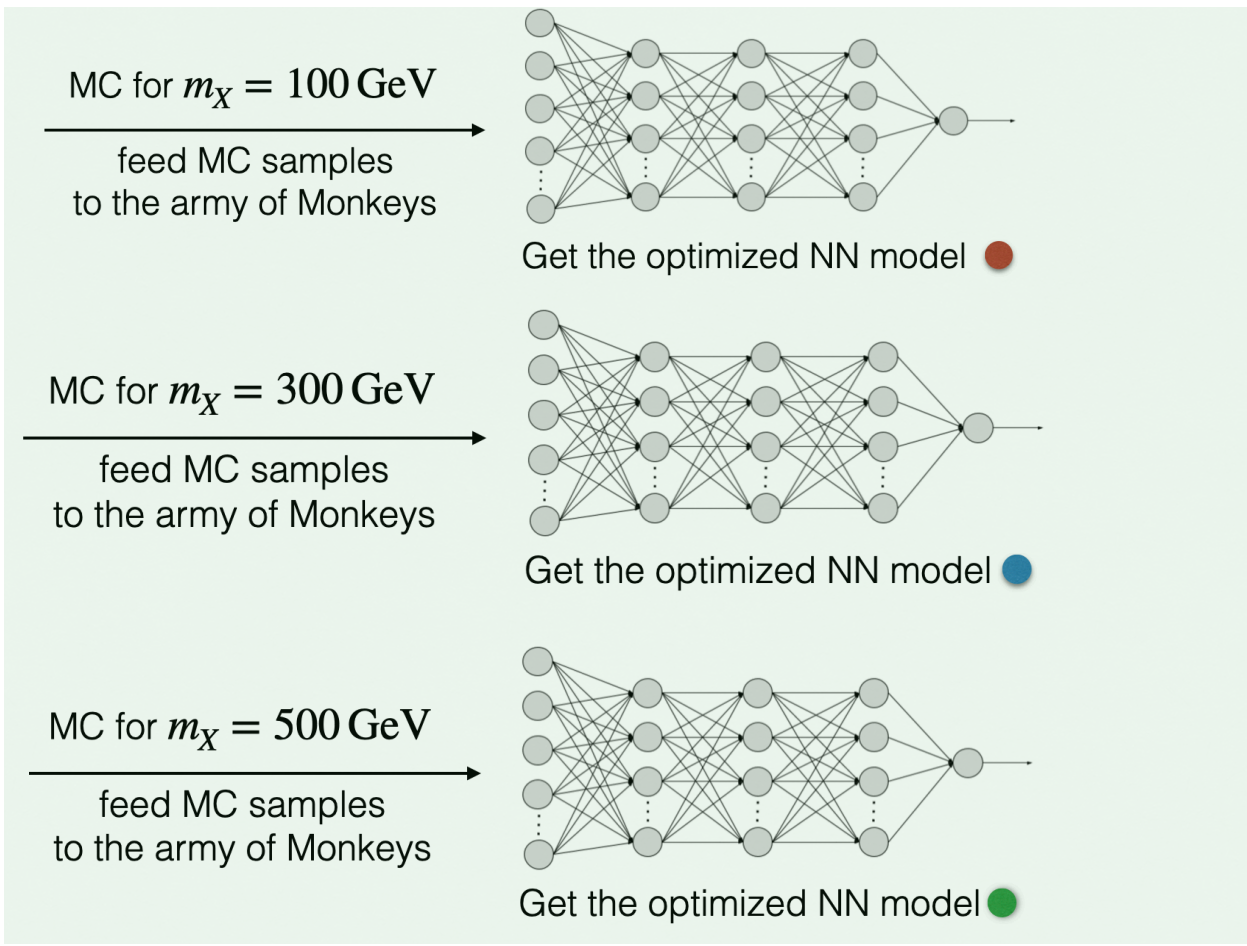
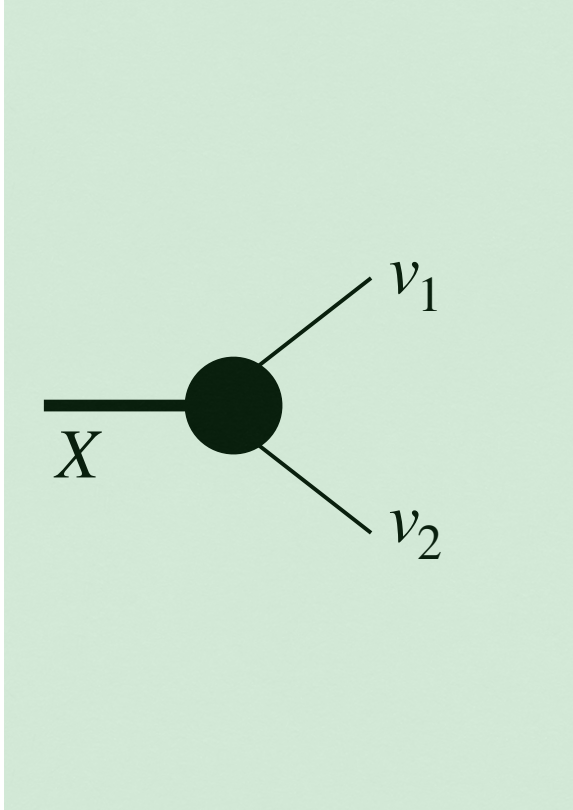


(= Save parameters of NN)

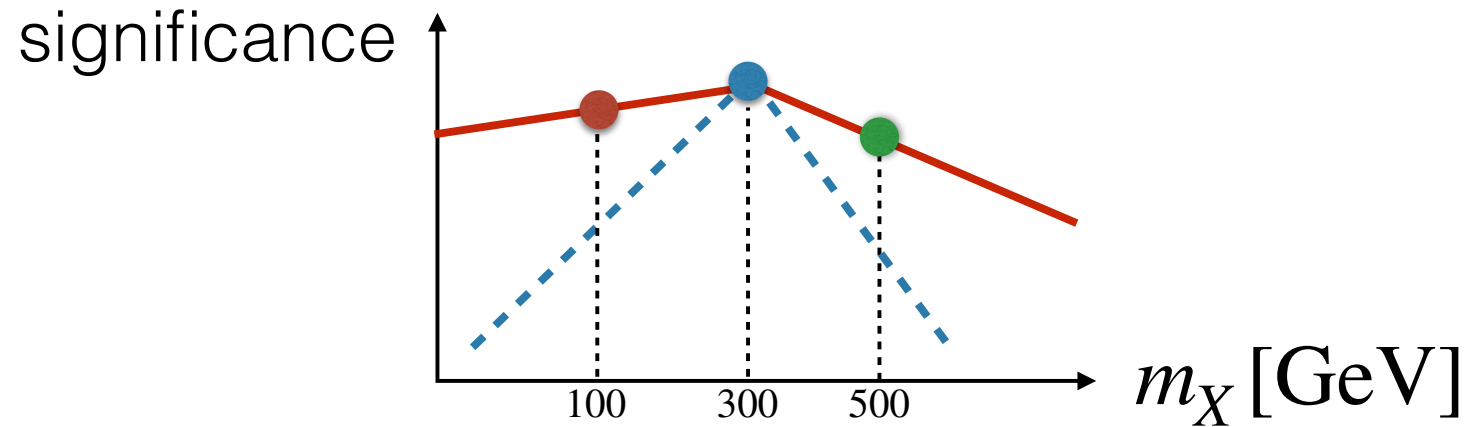
significance



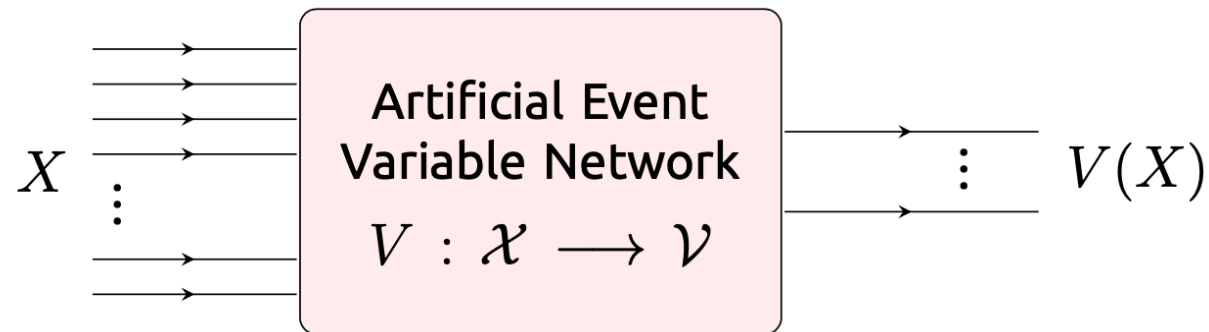
- Conventional supervised ML,



- Our **NN method** provide

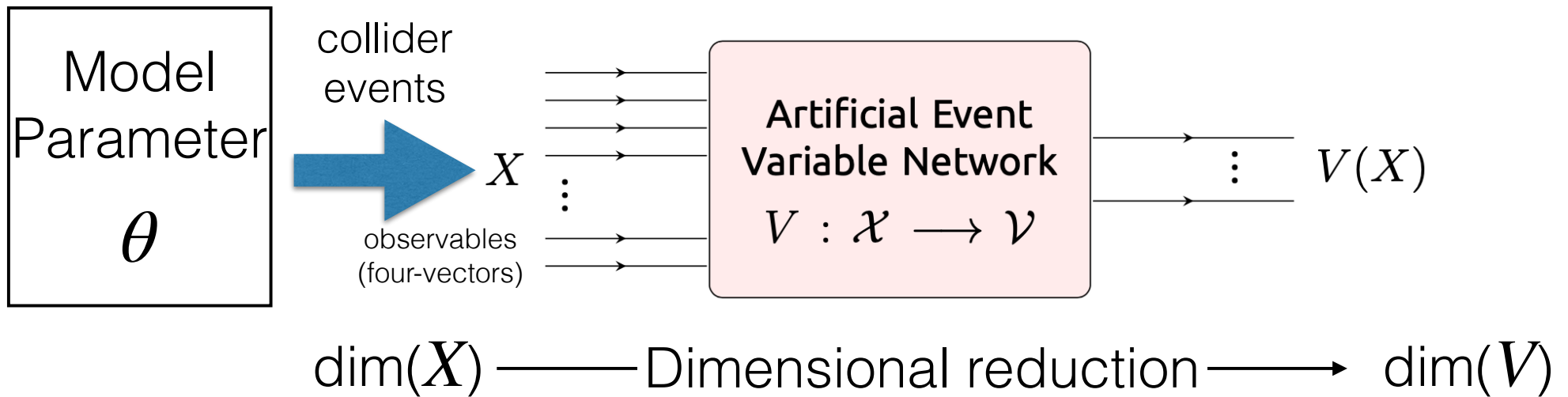


by synthesizing event variable with ML



- V is not signal vs background classifier

- We train the network so that V carries information about the underlying unknown parameter θ



- Some information would be lost due to $\dim(X) > \dim(V)$
 - Try to minimize the information loss
 - Efficiently retain the underlying parameters θ

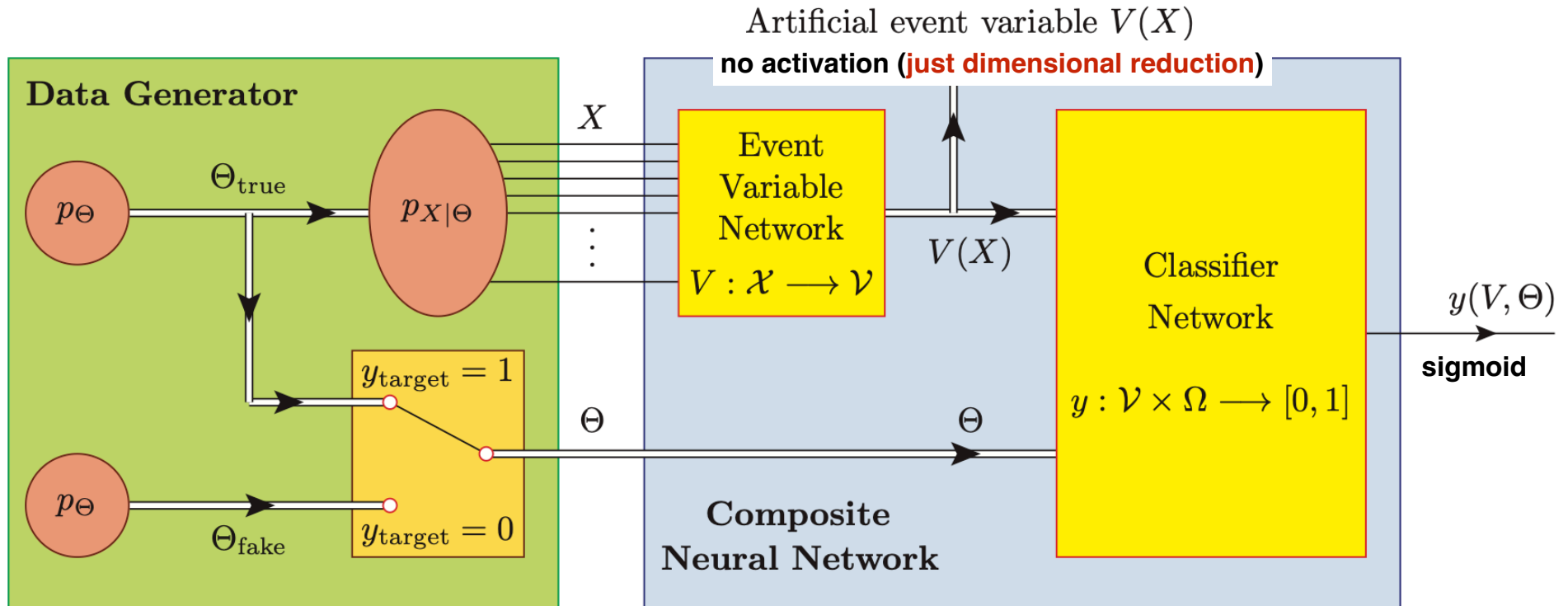
$$I(V; \Theta) = \int dv \int d\theta p_{V, \Theta}(v, \theta) \ln \left[\frac{p_{V, \Theta}(v, \theta)}{p_V(v) p_{\Theta}(\theta)} \right]$$

- This is KL divergence between $p_{(V, \theta)}$ and $p_V \otimes p_{\theta}$

Train V so that $p_{(V, \theta)}$ and $p_V \otimes p_{\theta}$ are highly distinguishable

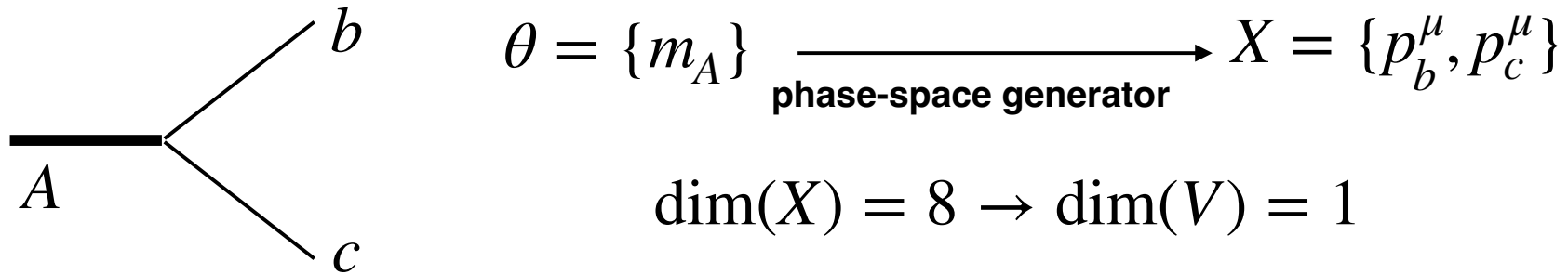
How to train V ?

- Use two classes
 1. $p_{X|\theta}$: events X **from** θ
 2. $p_X \otimes p_\theta$: events X **not from** θ (totally uncorrelated)

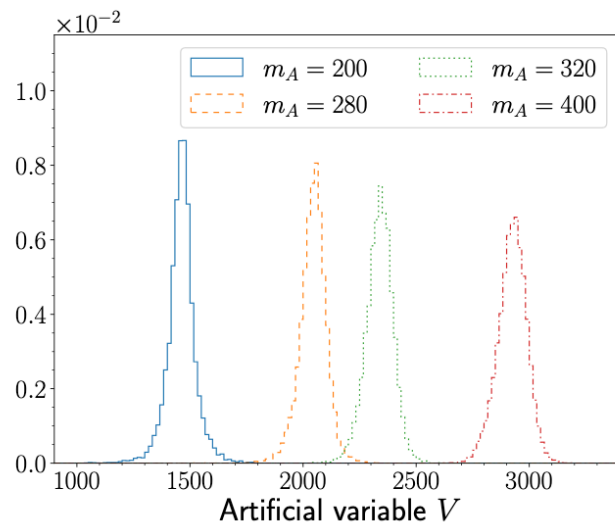


Does EV work?

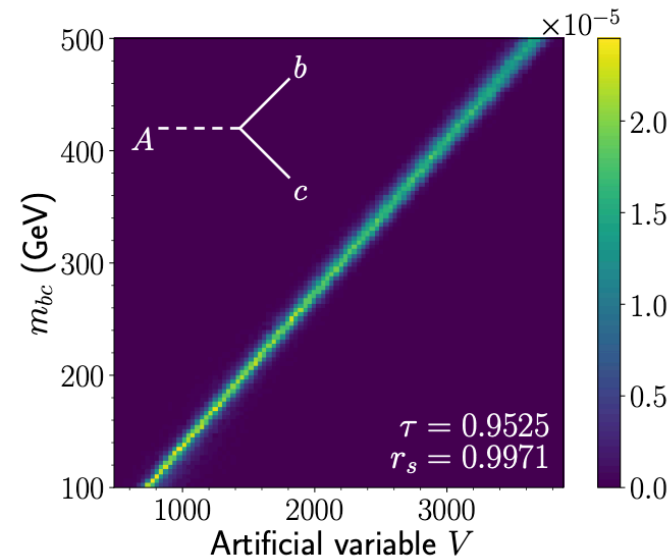
- Simplest example: Invariant mass



- Compare "Human-engineered EV = m_{bc} " and ML-EV



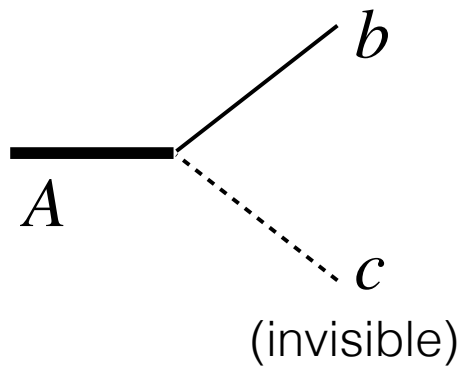
Event variable in action



What has the Machine learned?

Kendall's τ coefficient, Spearman's rank correlation r_s

- Next Simple example: Transverse mass

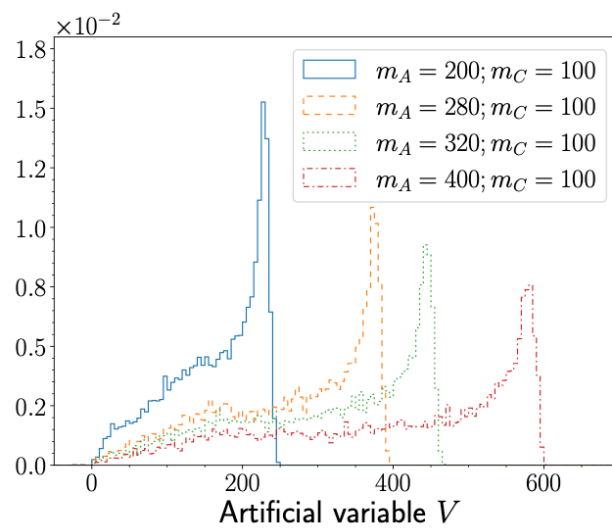


$$\theta = \{m_A\} \xrightarrow{\text{phase-space generator}} X = \{p_b^\mu, p_c^T\}$$

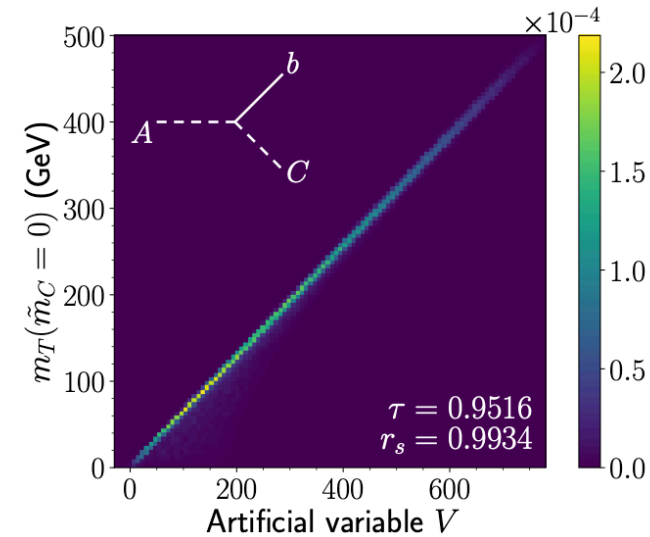
(No ISR, only beam-direction z -boost)

$$\dim(X) = 6 \rightarrow \dim(V) = 1$$

- Compare "Human-engineered EV = m_T " and ML-EV



Event variable in action



What has the Machine learned?

For Kinematics

- We have developed a **ML architecture** to find a "singular" variable to **describe a given kinematics** very well.
 - From now on, No human engineered feature variables required.
- what would be the next?

Orthogonal information to the Kinematics

- **Differences in radiation patterns of a Gauge charge** are coming from **"soft P_T " region** :Telling us about the state under a gauge group

Case of the Standard Model Gauge group

- In many cases, the **soft QCD radiation patterns** from signals are different from Backgrounds. (e.g. : rapidity gap)
- More detailed calculations on color flow and QCD dipole, arXiv:2407.04897 by Andrew Larkoski.

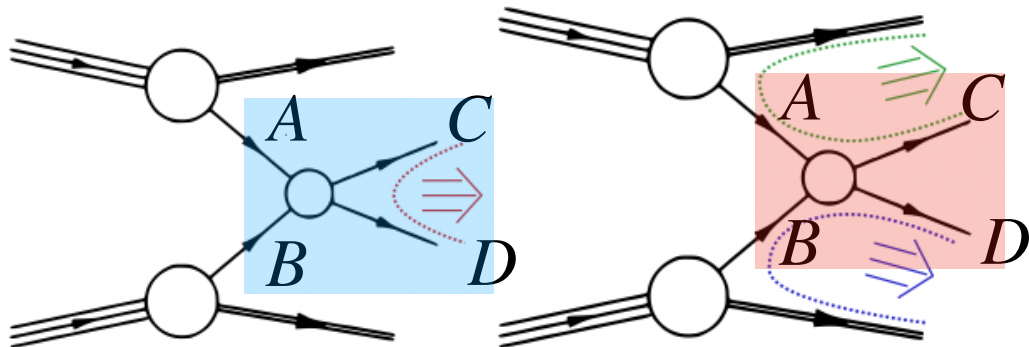
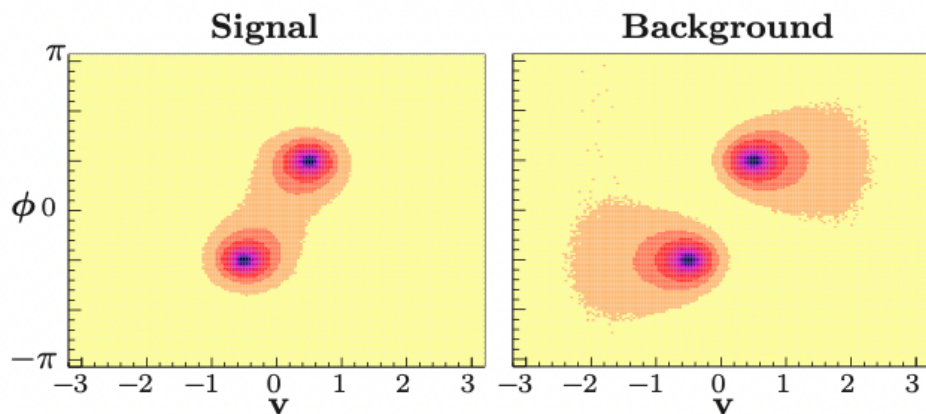


FIG. 1: Possible color connections for signal ($pp \rightarrow H \rightarrow b\bar{b}$) and for background ($pp \rightarrow g \rightarrow b\bar{b}$).



$$gg \rightarrow h \rightarrow b\bar{b}$$

$$\text{Tr}[T^A T^B] \text{Tr}[T^C T^D]$$

V . S .

$$gg \rightarrow b\bar{b}$$

$$\text{Tr}[T^A T^C] \text{Tr}[T^B T^D]$$

$$\text{Tr}[T^A T^D] \text{Tr}[T^B T^C]$$

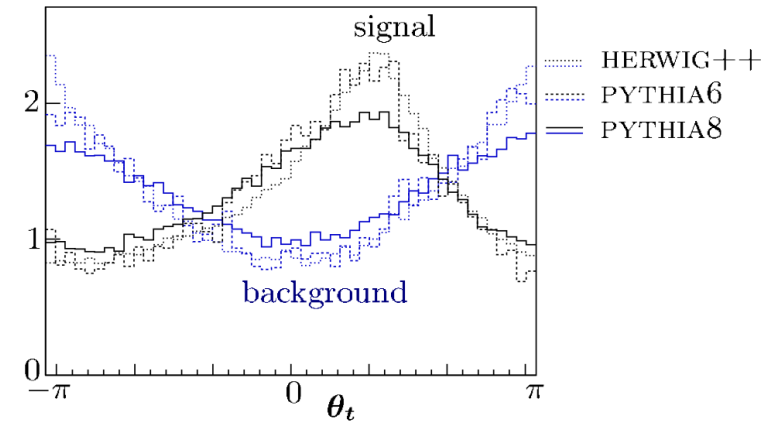
Utilizing localized information

- One can design a QCD variable, for example a pull-vector

$$\vec{t} \equiv \sum \frac{p_T^i |r_i|}{p_T^{\text{jet}}} \vec{r}_i$$

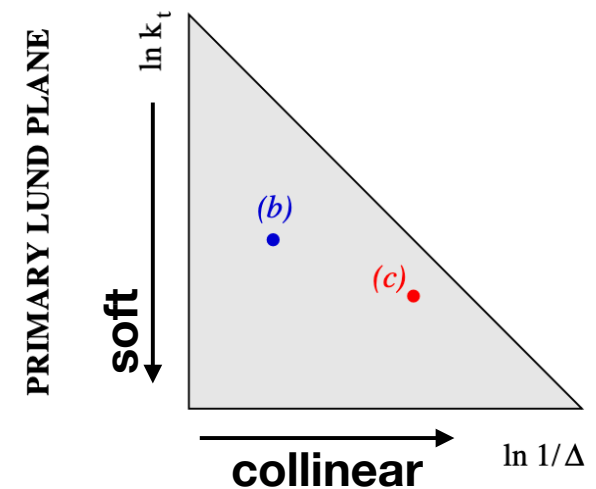
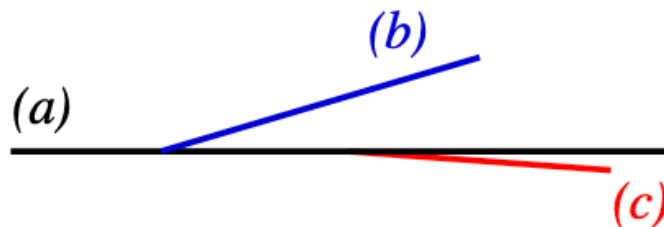
(Jason Gallicchio, Matthew D. Schwartz 2010)

provides an one-dimensional feature



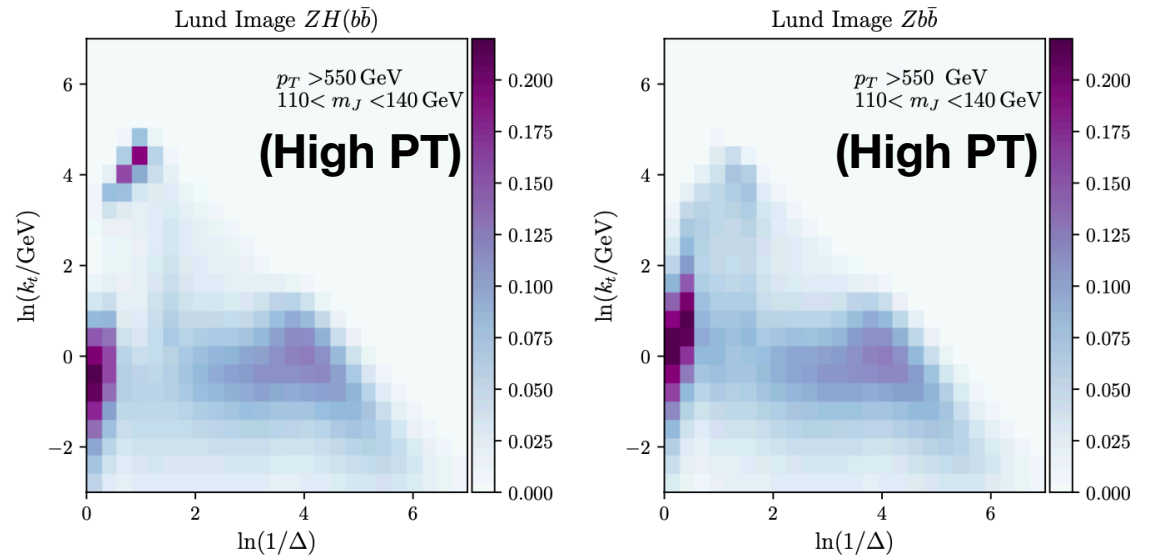
- Or one can get two-dimensional features,

(Frederic A. Dreyer, Gavin P. Salam, Gregory Soyez 2018)

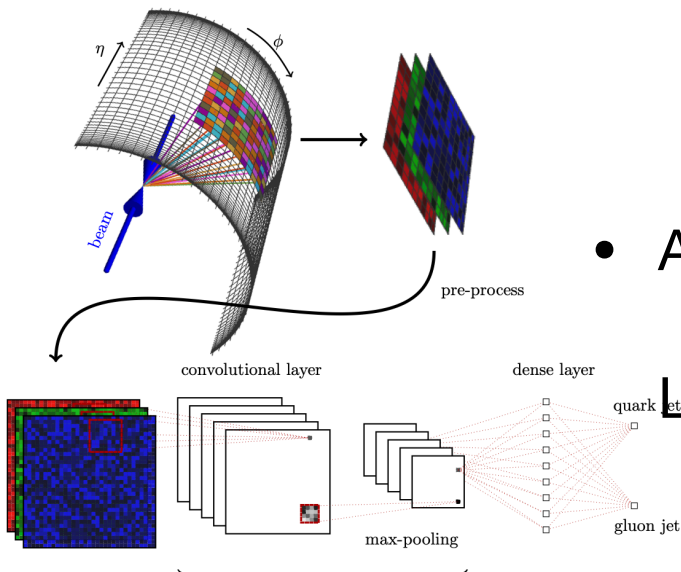


Fully utilizing localized information

- One needs to understand **differences** in "the full information"



(Charanjit K. Khosa, Simone Marzani, 2021)



M. Schwartz et.al. (JHEP 2017)

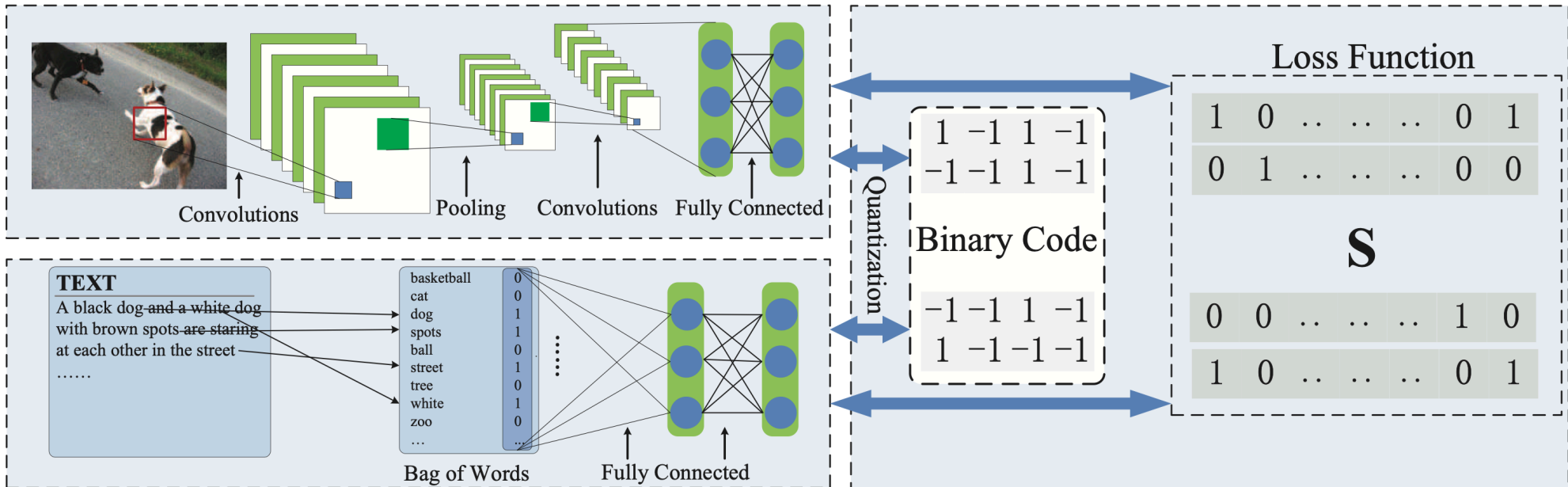
- A **neural network** can tell differences using pixels

Low level information \rightarrow feature engineering \rightarrow NN

Combining two different information



Multi-modal Network

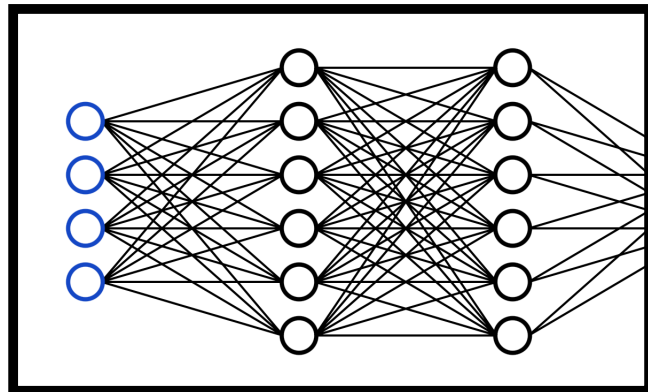
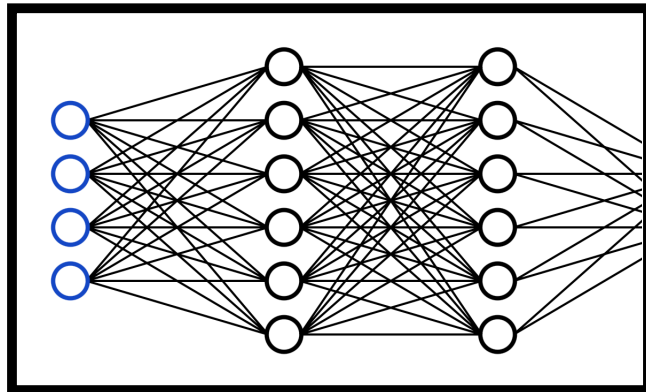


- In the commercial applications of Machine Learning, various sources of information (for example, different images, text) are utilized to interpret a situation in a consistent way.
- Here, we take the concept of Multi-modal Network
 - to extract (1) local features from QCD activities
 - (2) global features from Kinematics
 - and to combine these two streamline.

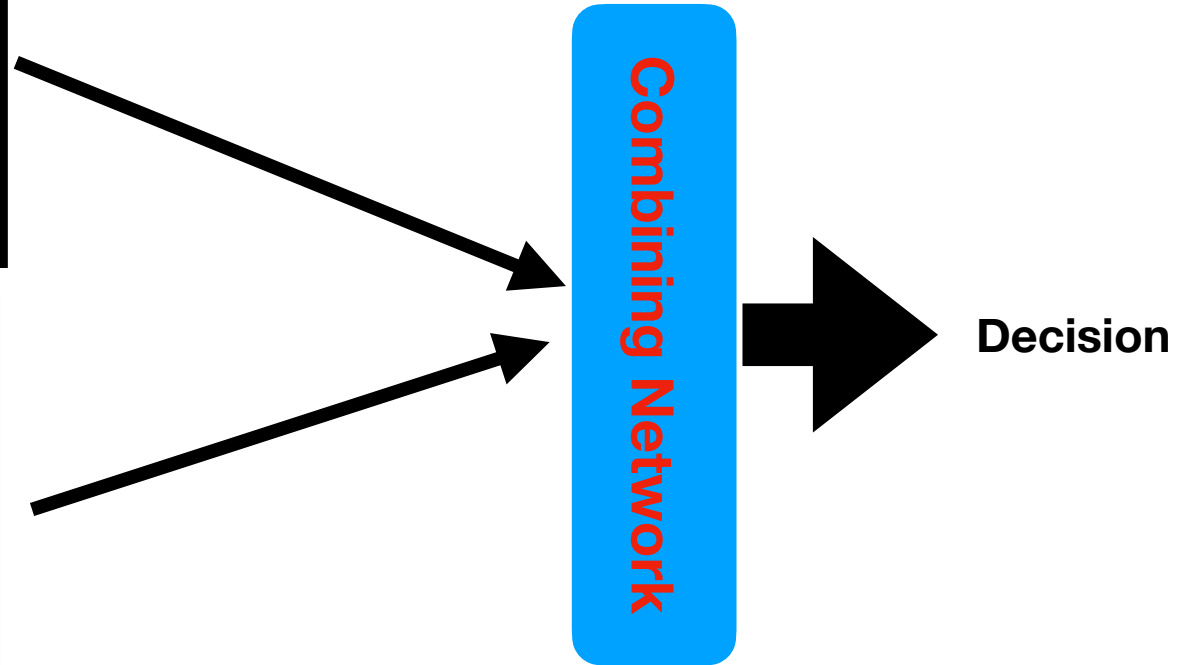
Global and Local information

- Separate Neural Network during information bottleneck process
- Combination layer before decision

A Neural Network for "Global" information (kinematics)

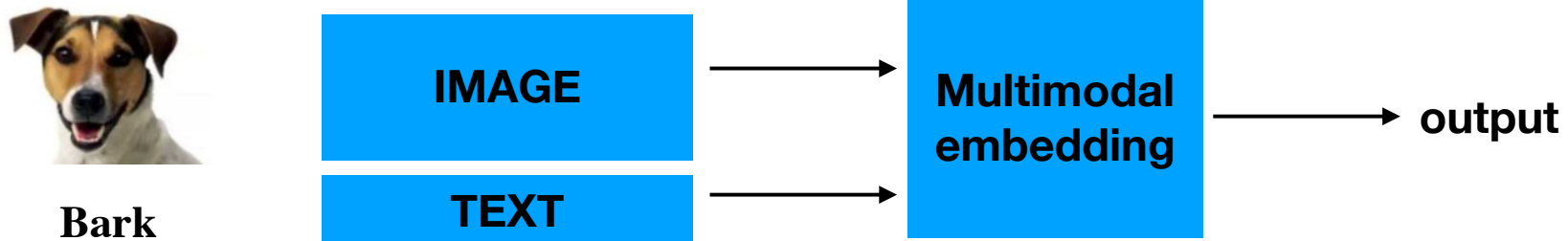
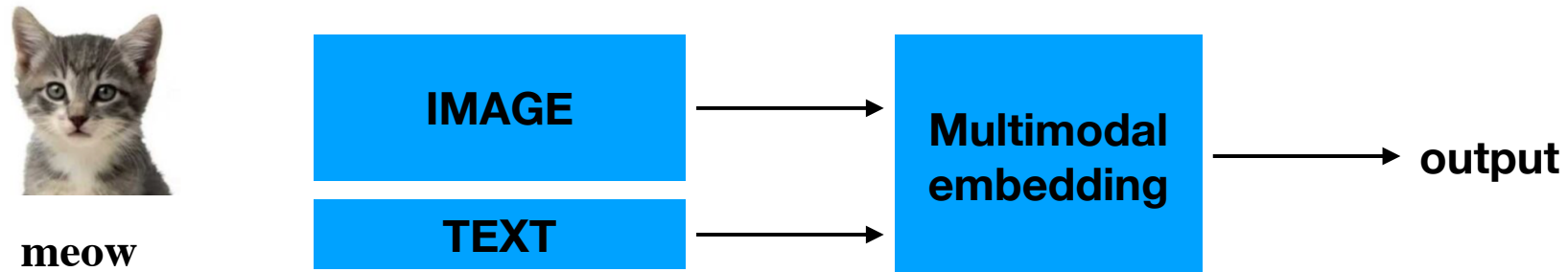


A Neural Network for "localized" information (QCD activities)



Multi-modal Network in conventional applications

- Commercial Multi-Modal application to enhancing the accuracy through **consistent** patterns **across modalities**



Multi-modal Network in collider physics

- In the collider physics, "kinematics" and "localized pattern" (for example QCD) are **orthogonal information**, so that we need to take a **complementary** approach.



meow

IMAGE

TEXT



Multimodal embedding



output



Bark

IMAGE

TEXT



Multimodal embedding



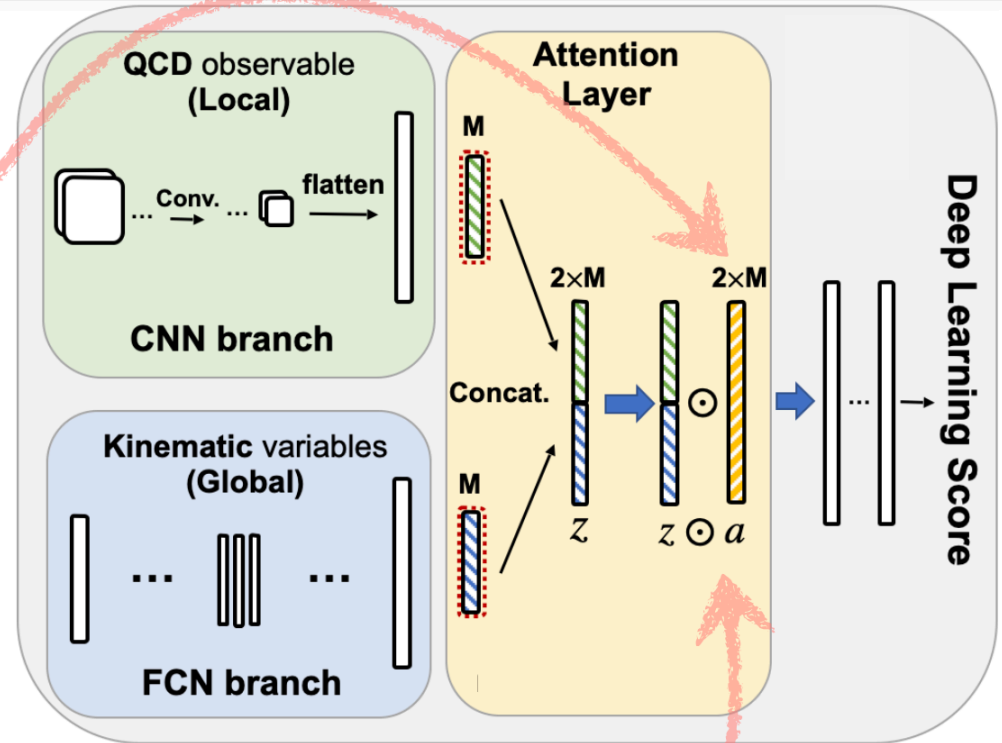
output



Attention mechanism inspired by NLP

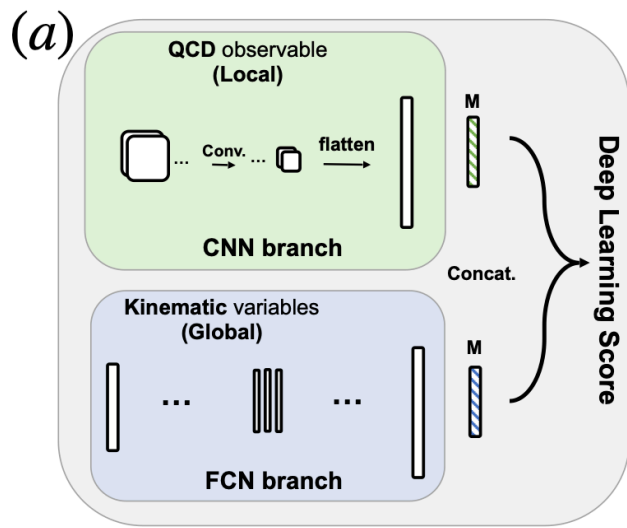
Attention score $\rightarrow a(z) = \frac{e^{J_{attn}(z)}}{\sum_{j=1}^{2M} e^{f_{attn}(z)_j}}$

where the layer $z = [z_{1:M} : z_{M+1:2M}]$ which is the concatenated layer from **CNN** and **FCN** respectively, and $f_{attn}(x) = W_{attn}x + b_{attn}$ is a trainable linear transformation.

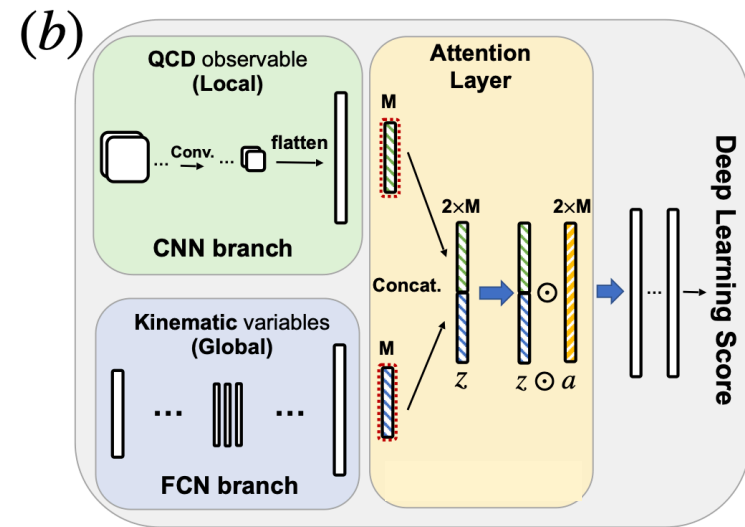


Attention value $\rightarrow z \odot a$

- ✓ The **attention values** are computed as Hadamard product between the attention score (a) and the concatenated layer (z).
- ✓ We can interpret how much the model concentrates the two base models to classify signal and background.
- ✓ Attention values are then connected with a fully connected layer for classification.



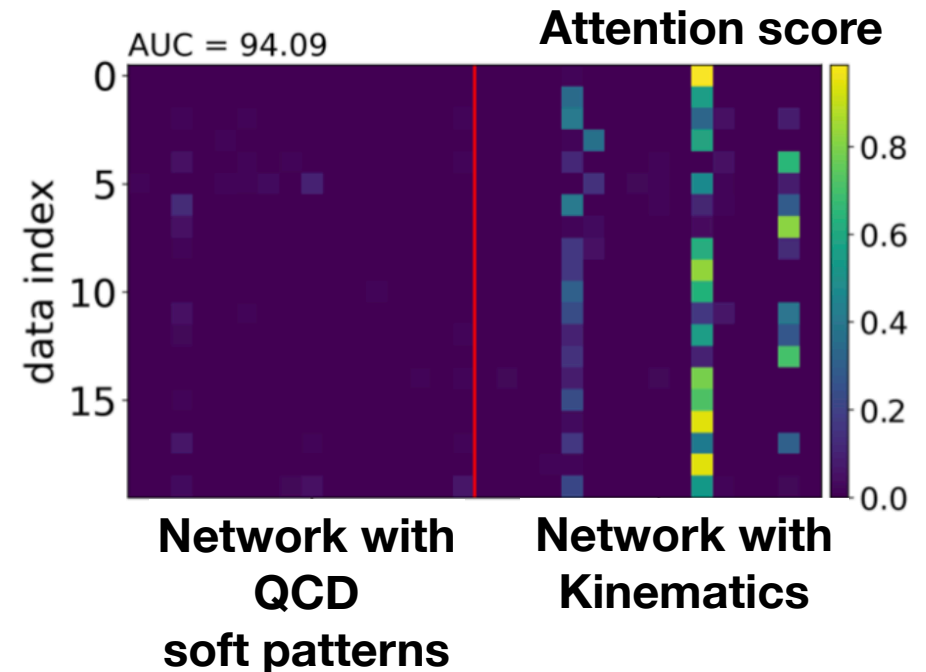
**Conventional
Black-box NN**

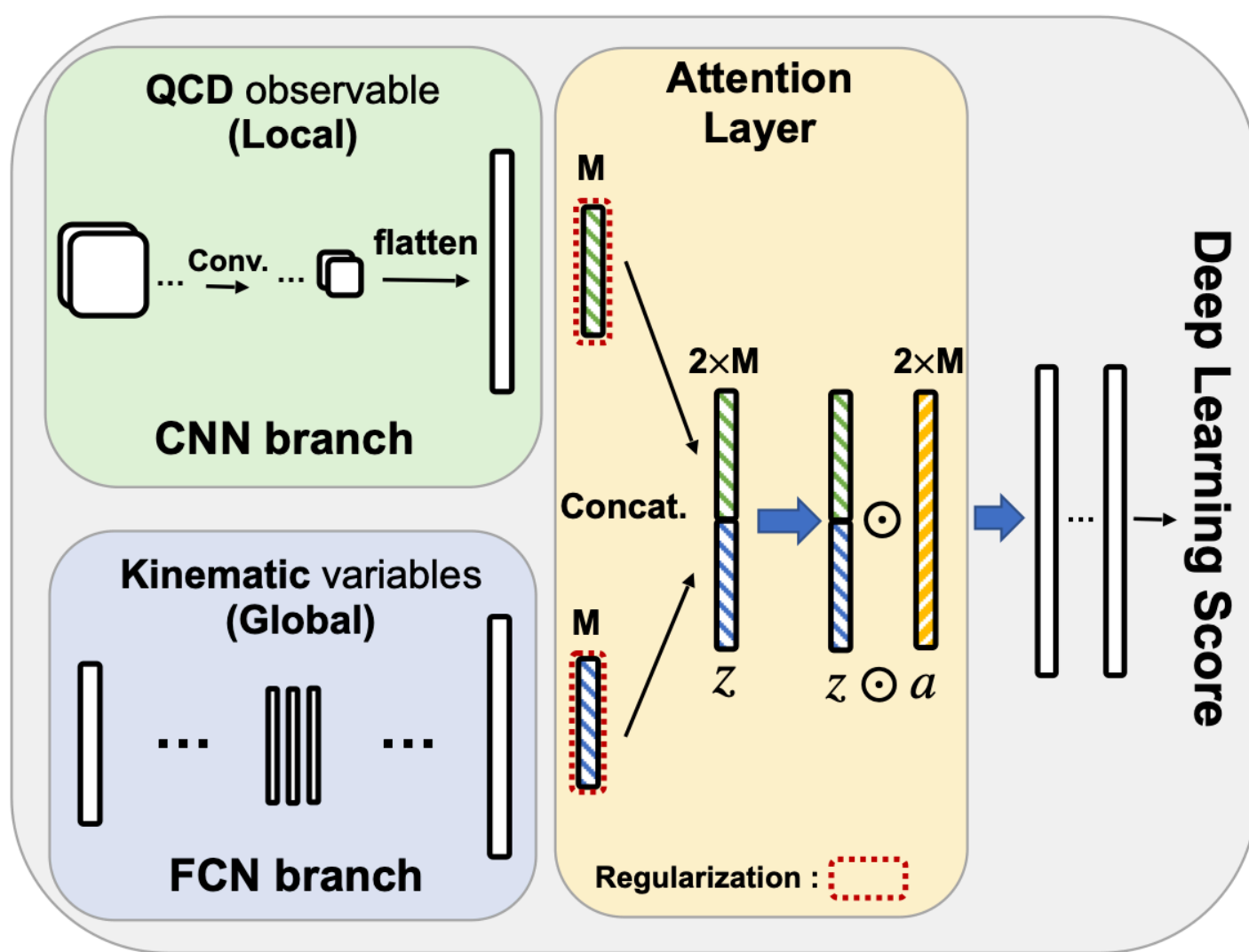


Transparent NN

- With an attention layer,
we can observe that

Network with the conventional combination **focus mostly on the easier material to study. (kinematics)**





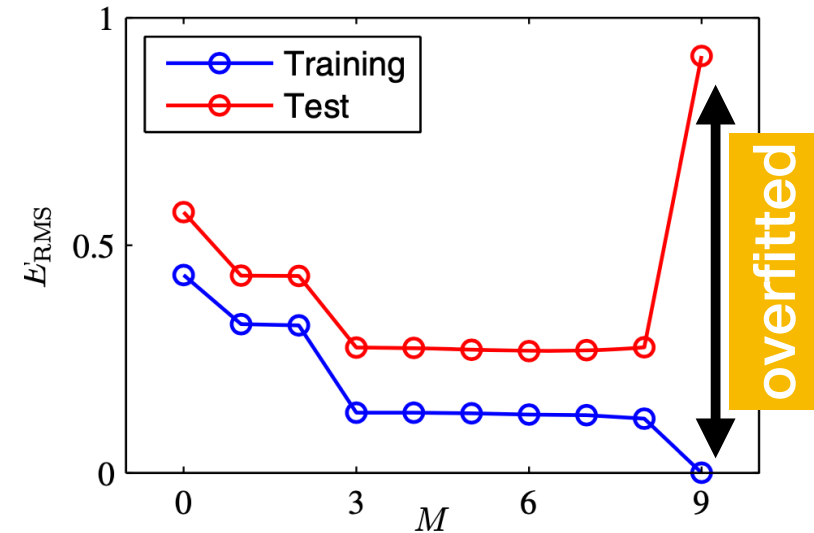
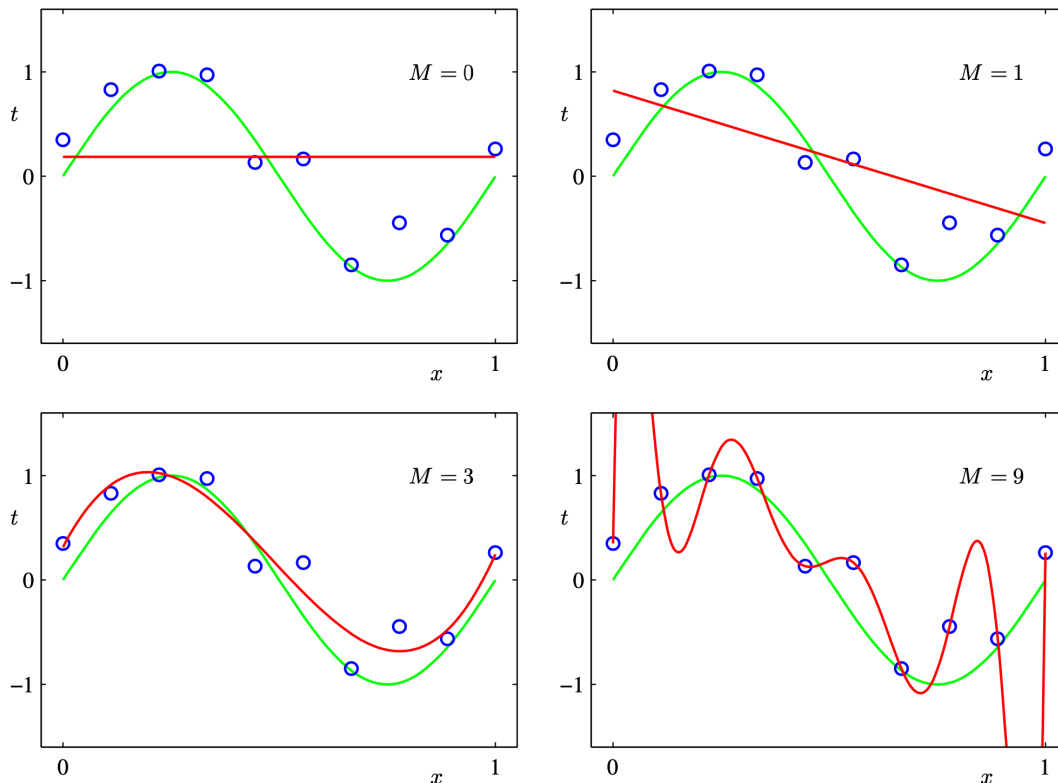
$$\text{Regularization term} = l_2 \times \sum_{k=1}^M W_k^2 \quad \mathcal{O}(10^{-2})$$

Actually, this is related to the **core** of ML

- protecting overfitting

- With complicated networks, the overfitting can occur !

$$y(x, \omega) = \omega_0 + \omega_1 x + \omega_2 x^2 + \dots + \omega_M x^M$$

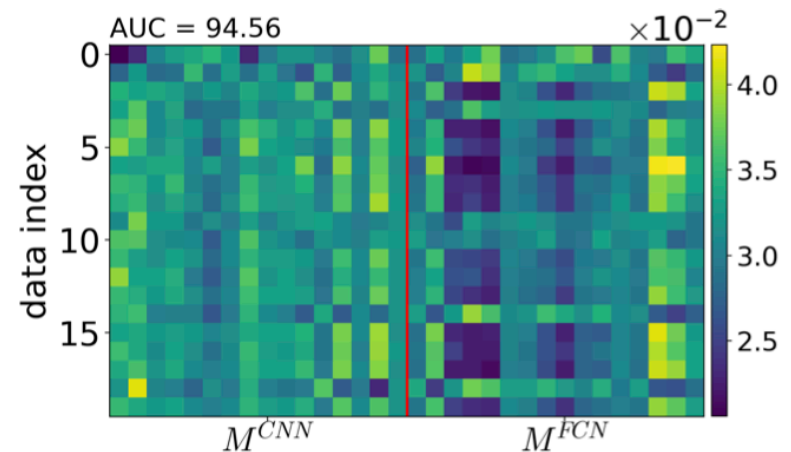
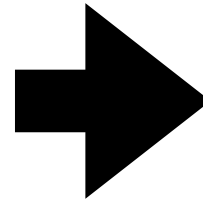
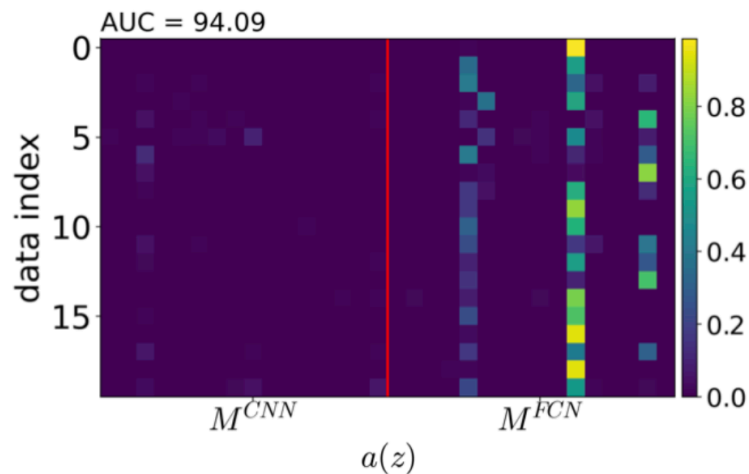


	$M = 0$	$M = 1$	$M = 6$	$M = 9$
w_0^*	0.19	0.82	0.31	0.35
w_1^*		-1.27	7.99	232.37
w_2^*			-25.43	-5321.83
w_3^*			17.37	48568.31
w_4^*				-231639.30
w_5^*				640042.26
w_6^*				-1061800.52
w_7^*				1042400.18
w_8^*				-557682.99
w_9^*				125201.43

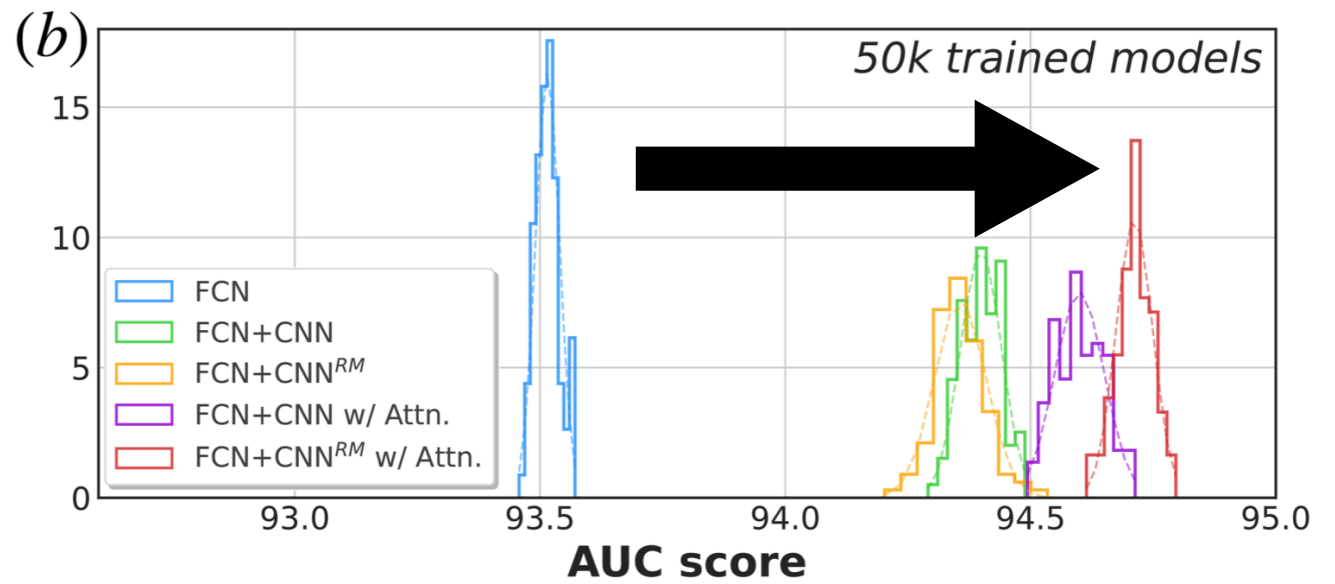
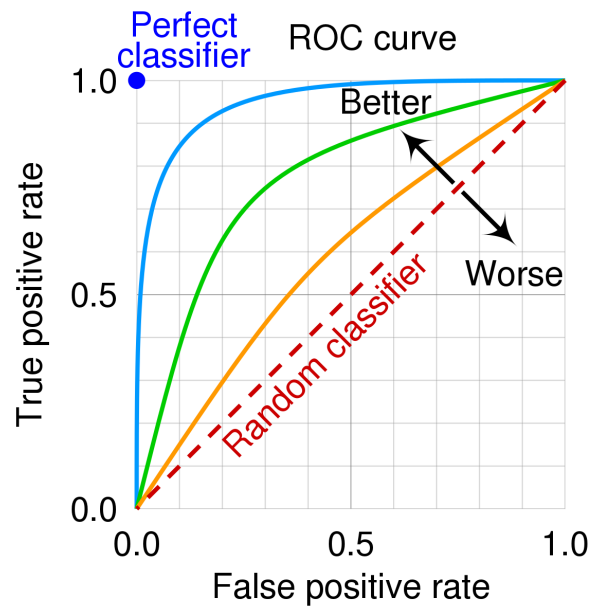
- Utilize a **regularizer**, a "**Lagrangian Multiplier**" in ML

$$\text{Regularization term} = l_2 \times \sum_{k=1}^M W_k^2$$

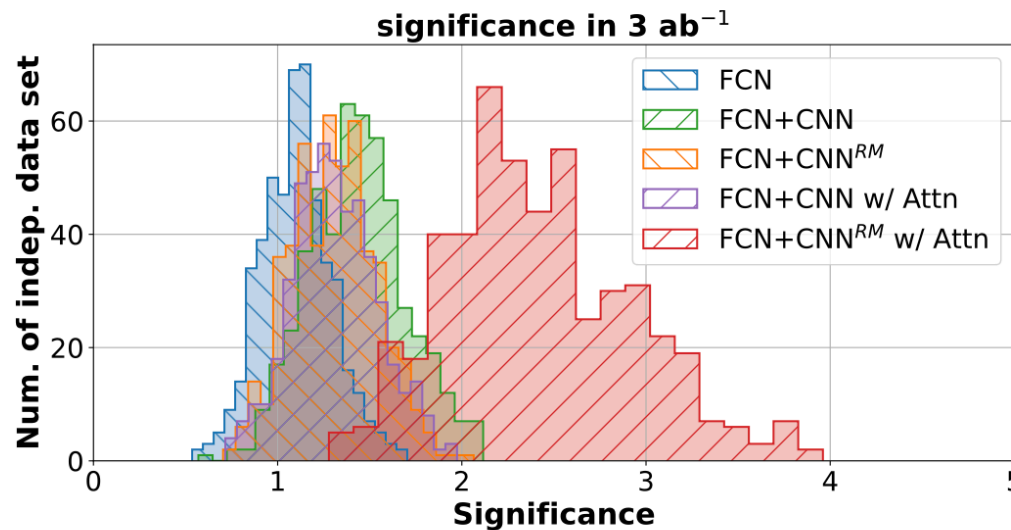
- this **simple technique** works to **balance** information between local and global information!



- A simple but effective solution.



- AUC score is the area under the ROC curve.
Perfect discrimination = AUC score=100
- We get the improvement in the performance as a result.



AI for Collider Physics

- **Efficient parameter exploration**
 - Precision measurements impose increasingly complex constraints on theory parameter spaces.
 - AI helps us efficiently explore the surviving regions consistent with experimental data.
- **Efficient Monte Carlo simulation**
 - As collider measurements become more precise, theoretical predictions must keep pace.
 - AI-assisted Monte Carlo techniques improve the precision and efficiency of theoretical calculations.
- **Enhanced new-physics discovery**
 - New physics signals can be subtle and distributed across multiple observables.
 - AI can combine complementary information more effectively, improving the sensitivity of collider searches.